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(54) Herpesviral proteases, compositions capable of binding them and uses thereof.

(57) Novel herpes viral protease crystalline structures are identified which have an active site formed by the three amino acids Ser, His and His. Also disclosed are methods of identifying inhibitors of these proteases and/or active sites.

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Description

Technical Field of the Invention

- 5 The invention relates to the identification of a novel protease catalytic active site and methods for enabling the design and selection of inhibitors of proteases, esterases, ligases and other hydrolases with that active site.

Background of the Invention

- 10 Herpesviridae is a family of envelope DNA viruses comprising three subfamilies, alpha, beta and gamma herpesviridae. The alpha subfamily includes herpes simplex virus (HSV) 1 and 2, and varicella zoster virus (VZV). The beta subfamily includes cytomegalovirus (CMV) and human herpes virus 6 (HHV-6) and human herpes virus 7 (HHV-7). The gamma subfamily includes Epstein-Barr virus (EBV) and human herpes virus (HHV-8).

- 15 The human herpes viruses are responsible for a variety of disease states from sub-clinical infections to fatal disease states in the immunocompromised. As one example, VZV is known to cause a number of serious diseases: chickenpox, shingles and post-herpetic neuralgia [S. Straus, *Ann. Neurol.*, 35:S11-S12 (1994)]. As another example, HSV-1 is acquired in childhood when it causes a self-limiting gingivostomatitis. The virus remains latent in the dorsal root ganglia and is reactivated later in life as cold sores in about one third of the population. HSV-1 is also a cause of keratitis, resulting in more than 300,000 cases per year in the US. HSV-2 is usually acquired through sexual contact and gives
20 rise to genital herpes. Human CMV is a ubiquitous opportunistic pathogen that can result in life threatening infections in congenitally infected infants, immunocompromised individuals and immunosuppressed cancer and transplant patients.

- Each of these members of the herpes virus families encodes a serine protease that is essential for its replication [F. Liu, & B. Roizman, *J. Virol.*, 65:5149-5156 (1991) (Liu I); F. Liu & B. Roizman, *Proc. Natl. Acad. Sci.* 89: 2076-2080 (1992) (Liu II); F. Liu & B. Roizman, *J. Virol.*, 67: 1300-1309 (1993) (Liu III); A. R. Welch *et al.*, *J. Virol.*, 67: 7360-7372 (1993) (Welch I); E. Z. Baum *et al.*, *J. Virol.*, 67: 497-506 (1993); J. T. Stevens *et al.*, *Eur. J. Biochem.*, 226: 361-367 (1994); A. R. Welch *et al.*, *J. Virol.*, 69: 341-347 (1993) (Welch II); D. L. Hall & P. L. Darke, *J. Biol. Chem.*, 270: 22697-22700 (1995); Weinheimer *et al.*, *J. Virol.*, 67: 5813-5822 (1993); M. Gao *et al.*, *J. Virol.*, 68: 3702-3712 (1994); C. L. Dilanni *et al.*, *J. Biol. Chem.*, 268: 25449-25454 (1993) (Dilanni I); C. L. Dilanni *et al.*, *J. Biol. Chem.* 269: 12672-12676 (1994) (Dilanni II); P. J. McCann III *et al.*, *J. Virol.*, 68: 526-529 (1994)]. These proteases each provide a potential target
30 for therapeutic intervention.

- The proteases from these viruses are encoded as precursor proteins that catalyze their own cleavage to produce an N-terminal domain of approximately 28 kDa having full or increased catalytic activity. These protease domains show some degree of sequence homology - 20% to 40% identity between members of different subfamilies and as high as
35 90% identity within each subfamily. They show little sequence homology to any other known protein, including the absence of the conserved G-X-S/C-G-G [SEQ ID NO: 12] for chymotrypsin-like and G-T-S-M/A [SEQ ID NO: 13] for subtilisin-like proteases. The known herpes virus proteases all cleave a peptide bond between an alanine and a serine, but their substrate specificity beyond the scissile bond are different [A. Welch *et al.*, *J. Virol.* 69, 341-347 (1993)].

- Each known serine protease has its characteristic set of functional amino acid residues arranged in a particular
40 three dimensional configuration to form an active site. Knowledge of the active site of such proteases and their three dimensional structure permits the use of methods of structure-based drug design to identify and develop inhibitors of the proteases [C. Verlinde and W. Hol, *Structure*, 2:577-587 (July 1994); I. D. Kuntz, *Science*, 257:1078-1082 (August 1992)]. Because the proteolytic activity of the herpesvirus-encoded protease plays an essential role in virus capsid maturation, inhibitors of the protease would thus inhibit infectious virus particle formation and thereby exert an antiviral
45 action. For serine proteases of which trypsin is a prototype, the active site is formed by Ser, His and Asp [H. Neurath, *Science*, 224: 350-357 (April 1984)]. These three residues are known as the catalytic triad.

- There is a need in the art for novel protease active sites and catalytic sequences to enable identification and structure-based design of protease inhibitors, which are useful in the treatment or prophylaxis of viral diseases caused by viruses of the herpes family, as well as other diseases in which the target enzyme may share catalytic domains with
50 those of the herpes family.

Summary of the Invention

- The present invention provides novel herpes protease crystalline forms. In one aspect, the present invention provides liganded and unliganded herpes HSV-2 protease, HSV-1 protease, CMV protease, and VZV protease crystalline forms, each of which is characterized by a three dimensional catalytic site formed by the three amino acid residues Ser, His, and His.

In another aspect, the present invention provides novel HSV-1 and HSV-2 protease compositions characterized by a three dimensional catalytic site of the seven amino acid residues, Ser 129, His 61, His 148, Ser 131, Cys 152, Arg

156, and Arg 157 of SEQ ID NOS: 3 and 4.

In still another aspect, the present invention provides a novel unliganded HSV-2 protease composition characterized by a three dimensional catalytic site of the seven amino acids identified above, and further containing amino acid residues Leu 27, Val 128, and Leu 130 of SEQ ID NO: 4; and optionally two water molecules Wat1 and Wat2 which are present in the liganded form.

In yet another aspect, the present invention provides an HSV-2 protease having an active site characterized by the coordinates selected from the group consisting of the coordinates of Figures 2 and 3, the coordinates of Figures 8 and 9, and the coordinates of Figures 11 and 12. In another aspect, the present invention provides an HSV-2 protease having an active site characterized by the coordinates selected from the group consisting of the coordinates of Figures 4 and 5, the coordinates of Figures 8 and 9, the coordinates of Figures 11 and 12, and the coordinates of Figures 14 and 15.

In yet a further aspect, the present invention provides a novel HSV-1 protease composition characterized by a three dimensional catalytic site of Ser 129, His 61, His 148, Ala 131, Cys 152, Arg 156 and Arg 157 [SEQ ID NO: 3]. In one embodiment, this HSV-1 protease has an active site characterized by the coordinates selected from the group consisting of the coordinates of Figure 6 or Figure 7, the coordinates of Figure 10; and the coordinates of Figure 16.

In still another aspect, the present invention provides a novel CMV protease composition characterized by a three dimensional catalytic site of four amino acid residues, Ser, His, His, and Asp. In one embodiment, the CMV protease active site is formed by at least the amino acids Ser 132, His 63, His 157, Asp 65, Cys 161 and Ser 134. In another embodiment, the CMV protease active site further contains at least one amino acid selected the group consisting of Arg 165 and Arg 166. Desirably, the CMV protease active site is characterized by the coordinates selected from the group consisting of Figure 17 or Figure 21, the coordinates of Figure 18 and the coordinates of Figure 20.

In yet another aspect, the present invention provides a novel CMV protease composition characterized by a three dimensional catalytic site of nine amino acid residues, Ser 132, His 63, His 157, Asp 65, Ser 134, Cys 161, Arg 165, Arg 166 and Asn 60.

In yet another aspect, the present invention provides a novel VZV protease composition characterized by a three dimensional catalytic site of four amino acid residues of SEQ ID NO: 5: Ser 120, His 52, His 139, and Lys 54. In another aspect, the VZV protease has a catalytic site which includes the four amino acids identified above and Ser 122, Cys 143, Arg 147 and Arg 148. In one embodiment, the VZV protease active site is characterized by the coordinates selected from the group consisting of Figure 22 or Figure 23, the coordinates of Figure 24 and the coordinates of Figure 26.

In another aspect, the present invention provides a heavy atom derivative of a herpes virus protease crystal, where the herpes virus protease is HSV1, HSV2, CMV, or VZV.

In a further aspect, the invention provides a method for identifying inhibitors of the compositions described above which methods involve the steps of: providing the coordinates of a protease structure of the invention to a computerized modeling system; identifying compounds which will bind to this structure; and screening the compounds or analogs derived therefrom identified for protease inhibitory bioactivity. In one embodiment of this aspect, the inhibitor binds to the dimeric interface of the protease molecule, or fragment thereof, of the invention.

In yet a further aspect, the present invention provides for an inhibitor of the catalytic activity of any composition bearing a catalytic domain described above. Desirably, the inhibitor disrupts the ability of the protease molecule to form a dimer.

Another aspect of this invention includes machine readable media encoded with data representing the coordinates of the 3D structure of a protease crystal of the invention, or of a catalytic site domain thereof.

In yet another aspect, the invention provides a computer controlled method for designing a ligand capable of binding to the active site domain of a herpes protease involving the steps of providing a model of the crystal structure of the active site domain of a herpes protease, analyzing the model to design a ligand which binds to the active site domain, and determining the effect of the ligand on the active site.

Other aspects and advantages of the present invention are described further in the following detailed description of the preferred embodiments thereof.

Brief Description of the Drawings

Fig. 1 provides an alignment of the amino acid sequences herpes proteases HHV-6 [SEQ ID NO: 2], CMV [SEQ ID NO: 1], EBV [SEQ ID NO: 6], HSV-1 [SEQ ID NO: 3], HSV-2 [SEQ ID NO: 4] and VZV [SEQ ID NO: 5]. Regions of α -helices and β -strands in the HSV-2 protease structure are indicated by A1 through A7, and B1 through B7, respectively.

Fig. 2A-2F provides the coordinates of the residues of the catalytic triad and other residues and water molecules in the active site of the diisopropyl phosphate (DIP)-liganded HSV-2 protease.

Fig. 3A-3E provides the coordinates of the residues of the catalytic triad and other residues and water molecules in the active site of unliganded HSV-2 protease.

Fig. 4A-4MMM provides the protein coordinates of the DIP-liganded HSV-2 protease crystalline structure of the

invention. Figure 2A-2F is included within Figure 4A-4MMM.

Fig 5A-5DDD provides the protein coordinates of the unliganded HSV-2 protease crystalline structure. Figure 3A-3E is included in Figure 5A-5DDD.

Fig. 6A-6B provides the coordinates of residues in the active site region of HSV-1 protease.

Fig. 7A-7DDD provides the protein coordinates of the HSV-1 protease crystalline structure of the invention. Figure 6A-6B is included within Fig. 7A-7DDD.

Fig. 8A-8X provides the distances (in Angstrom) between any protein residue that has an atom within a 5.5 Å radius of any atom of Ser 129 covalently bonded to the DIP in the DIP-liganded HSV-2 protease [SEQ ID NO: 4].

Fig. 9A-9I provides the distances (in Angstroms) between every two atoms that are within 5.0 Å of the active site residues of the unliganded HSV-2 protease.

Fig. 10A-10B provides the distances (in Angstroms) between every two atoms that are less than 5 Å from the active site of HSV-1 protease.

Fig. 11A-11LLL provides the bond angles (in degrees) between any atom of HSV-2/DIP-modified Ser 129 and any two protein residue atoms that are within a 5.5 Å radius of the DIP modified Ser 129 [SEQ ID NO: 4].

Fig. 12A-12Q provides the bond angles (in degrees) between interresidue atoms in the active site region near Ser 129, His 61 and His 148 of the unliganded HSV-2 protease [SEQ ID NO: 4].

Fig. 13A-13D provides the bond angles between interresidue atoms in the active site region near Ser 129, His 61 and His 148 of the HSV-1 protease of this invention [SEQ ID NO: 3].

Fig. 14 provides the dihedral angles of the active site formed by Ser 129, His 61 and His 148 of the DIP-liganded HSV-2 protease [SEQ ID NO: 4].

Fig. 15 provides the dihedral angles of the active site formed by Ser 129, His 61 and His 148 of the unliganded HSV-2 protease [SEQ ID NO: 4].

Fig. 16 provides the dihedral angles of the active site formed by Ser 129, His 61 and His 148 of the HSV-1 protease [SEQ ID NO: 3].

Fig. 17A-17E provide the protein coordinates near the active site region (at amino acid residues Ser 132, His63, Ser 134, Cys161, Arg165 and His157, and including Arg166) of the CMV protease [SEQ ID NO: 1] according to this invention.

Fig. 18A-18C provide the distances in Angstroms between every two atoms that are less than 5Å from the active site for CMV protease.

Fig. 19A-19D illustrate the bond angles between interresidue atoms that are within four Å apart in the active site region near Ser132, His63, His157 and Asp65 of the CMV protease [SEQ ID NO: 1] according to this invention.

Fig. 20 provides the dihedral angles of the tetrad active site formed by Ser132, His63, His157 and Asp65 of the CMV protease [SEQ ID NO: 1].

Fig. 21A-21DD provides the protein coordinates of the CMV protease crystalline structure of the invention. Fig. 17A-17E is included within Fig. 21A-21DD.

Fig. 22A-22C provide the protein coordinates near the active site region (at amino acid residues Ser 120, Ser 122, His 52, Lys 54, Cys 143, Arg 147 and Arg 148 of SEQ ID NO: 5) of the VZV protease according to this invention. The data is reported in Protein Data Bank (PDB) format as in Figs. 3A-3E.

Fig. 23A-23SS provide the protein coordinates of the VZV protease crystalline structure of the invention, including the active site of Figure 22A-22C.

Fig. 24A-24C provide the distances in Angstroms between every two atoms that are less than 5Å from the active site for VZV protease.

Fig. 25A-25D illustrate the bond angles between interresidue atoms that are within four Å apart in the active site region near Ser 120, His 52 and His 139 of the VZV protease [SEQ ID NO: 5] according to this invention.

Fig. 26 provides the dihedral angles of the tetrad active site formed by Ser 120, His 52 and His 139 of the VZV protease [SEQ ID NO: 5].

Fig. 27A is a three dimensional ribbon diagram of the DIP-liganded HSV-2 protease dimer. The ligand diisopropyl phosphate (DIP) is shown in the active site of each monomer rendered in space filling models. The amino terminus is indicated by N. The drawing was produced using the program RIBBONS [Carson, M. *J. Mol. Graphics* 5, 103-106 (1987)].

Fig. 27B is the same structure as in Fig. 27A, viewing from 90° away.

Fig. 27C is the unliganded dimer. The structure is essentially identical to that of the DIP-liganded HSV-2 protease structure.

Fig. 28A is a three dimensional ribbon diagram of the HSV-1 protease dimer. The amino terminus is indicated by N. The drawing was produced using the program RIBBONS [Carson, M. *J. Mol. Graphics* 5, 103-106 (1987)].

Fig. 28B is the same structure as in Fig. 28A, viewing from 90° away.

Fig. 29A is a three dimensional diagram of the HSV-2 protease monomer. The ligand DIP is shown in the active site rendered as a space filling model. The amino terminus is indicated by N. The drawing was produced using the program RIBBONS [Carson, M. *J. Mol. Graphics* 5, 103-106 (1987)].

Fig. 29B is the same structure as in Fig. 29A, viewing from 90° away.

Fig. 29C is the unliganded HSV-2 monomer. The structure is the same as the DIP-liganded HSV-2 protease structure.

Fig. 30A is a three dimensional diagram of the HSV-1 protease monomer. The amino terminus is indicated by N. The drawing was produced using the program RIBBONS [Carson, M. *J. Mol. Graphics* 5, 103-106 (1987)].

Fig. 30B is the same structure as in Fig 30A, viewing from 90° away.

Fig. 31 is a topology diagram of the HSV-2 monomer of Fig. 29A and HSV-1 monomer of Fig. 30A with helices (A1 through A7) represented as cylinders, strands (B1 through B7) represented as arrows and termini as N or C. Strands B5 and B7 are next to each other. Amino acid positions are indicated.

Fig. 32A is a three dimensional diagram of the structure of CMV protease with the core β -barrel highlighted. The amino and carboxyl-termini are indicated by N and C. Disordered portions of the structure are represented by dashed lines. The diagram was drawn with the program MOLSCRIPT [P. Kraulis, *J. Appl. Crystallogr.*, 24: 946-950 (1991)].

Fig. 32B is the same structure as in Fig. 32A, viewing from 90° away.

Fig. 33A is a three dimensional diagram of the structure of VZV protease with the core β -barrel highlighted in two shades of gray. The amino and carboxyl-termini are indicated by N and C. A disordered portion of the structure is represented by a dashed line. The diagram was drawn with the MOLSCRIPT program [P. Kraulis, *J. Appl. Crystallogr.*, 24:946-950 (1991)].

Fig. 33B is the same structure as in Fig. 33A, viewing from 90° away.

Fig. 34 is a topology diagram of the CMV monomer of Fig. 32A with helices (A1 through A7) represented as cylinders, strands (B1 through B7) represented as arrows and termini as N or C. Strands B5 and B7 are next to each other. Amino acid positions are indicated.

Fig. 35 is a topology diagram of the VZV monomer of Fig. 33A with helices (AA through A7) represented as cylinders, strands (B1 through B7) represented as arrows and termini as N or C. Strands B5 and B7 are next to each other. Amino acid positions are indicated.

Fig. 36A is a three dimensional diagram of the CMV protease dimer, viewing perpendicular to the two-fold axis, which was drawn using the MOLSCRIPT program.

Fig. 36B is the dimer of Fig. 36A, viewing parallel to the two-fold axis. The two parallel helices are indicated by A6. The active site regions are represented by Ser at the Ser132 positions [SEQ ID NO: 1].

Fig. 37 is a three dimensional diagram of the VZV protease dimer, viewing parallel to the two-fold axis, which was drawn using the MOLSCRIPT program, with each subunit in a different shade of grey.

Fig. 38A is a model of the DIP-liganded HSV-2 protease active site in a thick stick representation. All carbon atoms are in light shading; nitrogen, oxygen and sulfur atoms in dark shading. The catalytic residues are Ser 129, His 61 and His 148. Other residues of importance are Arg 156, Arg 157 and possibly Ser 131, Cys 152, Leu 27, Val 128, Leu 130 [SEQ ID NO: 4] and the two water molecules Wat1 and Wat2 shown as spheres. Hydrogen bonds between the residues in this active site are shown with dotted lines.

Fig. 38B is a superposition of the unliganded HSV-2 protease (dark) and the DIP-liganded HSV-2 protease (light) structures where the DIP ligand has been removed from the active site serine for clarity.

Fig. 38C is the superposition between the active site of DIP-liganded HSV-2 protease and that of the classical serine protease γ -chymotrypsin complexed with mono isopropyl phosphate (MIP). In light shading is the HSV-2 protease in the identical orientation as in Fig. 38A, and in dark shading are the γ -chymotrypsin active site residues. Labels are those of protease γ -chymotrypsin. Hydrogen bonding in the oxyanion hole of γ -chymotrypsin is shown.

Fig. 38D is the superposition of DIP-liganded HSV-2 protease with CMV protease, illustrating the similarities and differences between the active sites of these two enzymes. Hydrogen bonding is shown for CMV protease but labels are for HSV-2 protease.

Fig. 39A is the HSV-1 protease active site in a thick stick representation. All carbon atoms are in light shading; nitrogen, oxygen and sulfur atoms in dark shading. The catalytic residues are Ser129, His61 and His148 [SEQ ID NO: 3]. Other residues of importance are Arg 156, Arg 157 and possibly Ala 131 and Cys 152 [SEQ ID NO: 3]. Hydrogen bonds between the residues in this active site are shown with dotted lines.

Fig. 39B is the superposition between the active site of HSV-1 protease and that of the classical serine protease trypsin. In light shading is the HSV-1 protease in the identical orientation as in Fig. 39A, and in dark shading are the trypsin active site residues. Labels are shown for both the active site of trypsin (Ser 195, His 57, Asp 102) and HSV-1 protease (Ser 129, His 61, and His 148).

Fig. 39C is the superposition of HSV-1 protease with HSV-2 protease, illustrating the similarities and differences between the active sites of these two enzymes. In light shading is the HSV-1 protease in the identical orientation as in Fig. 39A, and in dark shading are the HSV-2 protease active site residues (numbering of the residues is identical between HSV-1 protease and HSV-2 protease).

Fig. 39D is the superposition of HSV-1 protease with CMV protease, illustrating the similarities and differences between the active sites of these two enzymes. In light shading is the HSV-1 protease in the identical orientation as in Fig. 39A, and in dark shading are the CMV protease active site residues.

Fig. 40A is a drawing of the VZV protease active site in ball-and-stick representation drawn with MOLSCRIPT program. All carbon atoms are in light shading; nitrogen, oxygen and sulfur atoms in dark shading. The catalytic residues are Ser 120, His 52 and His 139 of SEQ ID NO: 5. Other residues of importance are Arg 147, Arg 148 and possibly Ser 122 and Cys 143 of SEQ ID NO: 5. The postulated proton transfer pathway is shown by dashed lines.

Fig. 40B is the superposition between the active site of VZV protease and that of the classical serine protease trypsin. In light shading is the VZV protease in the identical orientation as in Fig. 40A, and in dark shading are the trypsin active site residues. Labels are those of trypsin. The proton transfer pathway in trypsin are depicted in dotted lines.

Fig. 41A is a drawing of the stereoview of the CMV protease active site in ball-and-stick representation drawn with MOLSCRIPT program. The catalytic residues are Ser132, His63, His157 and optionally Asp65 [SEQ ID NO: 1]. Other residues of importance are Arg 165, Arg 166 and possibly Ser 134 and Cys 161 [SEQ ID NO: 1]. The postulated proton transfer pathway is shown by dashed lines. The side chain of Arg165 is disordered in the structure and hence omitted in the drawing. H₂O is an ordered water molecule.

Fig. 41B is a stereoview of the superposition between the active site of CMV protease and that of the classical serine protease trypsin. The CMV protease is in the identical orientation as in Fig. 41A. Labels are those of trypsin. The proton transfer pathway in trypsin are depicted in dotted lines.

Fig. 42 provides the statistics of structure determination for HSV-2 protease.

Fig. 43 provides the data collection statistics for native and heavy atom derivatives of CMV protease.

Fig. 44 is a stereoview of the superposition between the Ca trace of VZV protease and that of the CMV protease.

The light color strand is the CMV protease and the dark color strand is the VZV protease. In spite of the limited sequence homology and apparent conformational differences in some helical or loop regions, the core b-barrel of the VZV protease superimposes quite well with that of the CMV protease. Excluding regions that are drastically different (> 4 Å), the root-mean-square (rms) difference is only 1.3 Å between 142 (60%) Ca atoms from VZV and CMV.

Fig. 45A is the complete sequence of the VZV construct H6(N)VZV [SEQ ID NO: 7] containing an authentic protease domain preceded at the amino-terminus by six histidine residues (underlined) followed by an enterokinase cleavage site (bold, underlined).

Fig. 45B is the complete sequence of the VZV construct LQA-H6(C) VZV [SEQ ID NO: 8] containing an authentic protease domain followed by six histidine residues (underlined).

Fig. 45C is the complete sequence of the VZV construct LQAS-H6(C) VZV [SEQ ID NO: 9] containing an authentic protease domain followed by a serine residue and six histidine residues (underlined).

Fig. 45D is the complete sequence of the VZV construct LQAS-12aa ext H6(C) VZV [SEQ ID NO: 10] containing an authentic protease domain followed by a serine residue, 12 residues normally found after the LQAS R-site (bold underlined) and six histidine residues (underlined).

Fig. 45E is the complete sequence of the VZV construct Δ9 LQAS-12 aa ext H6(C) VZV [SEQ ID NO: 11] containing an authentic protease domain deleted at the amino-terminus (first nine natural residues removed and Cys 10 replaced by Met) and followed at the carboxyl-terminus by a serine residue, 12 residues normally found after the LQAS R-site (bold underlined) and six histidine residues (underlined).

Detailed Description of the Invention

The present invention provides novel herpes virus family protease crystalline structures, novel herpes virus protease active sites, and methods of use of the crystalline forms and active sites to identify protease inhibitor compounds (peptide, peptidomimetic or synthetic compositions) characterized by the ability to inhibit binding to the active site of herpes proteases. The herpes virus protease compositions of the invention are characterized by a three dimensional active catalytic site of conserved amino acid residues, Ser, His, and His.

For HSV-1 and HSV-2 proteases, these residues are located at aa Ser 129, His 61 and His 148 of SEQ ID NO: 3 and 4, respectively. For CMV protease, these residues are located at aa Ser 132, His 63 and His 157 of SEQ ID NO: 1. For VZV protease, these residues are located at aa Ser 120, His 52, and His 139 of SEQ ID NO: 5.

The present invention further provides a novel HSV-2 protease composition characterized by a three dimensional active catalytic site of three conserved amino acid residues, Ser 129, His 61, His 148, seven additional amino acid residues Ser 131, Cys 152, Arg 156, Arg 157, Leu 27, Val 128, Leu 130, and two water molecules Wat1 and Wat2 (present in only the DIP-liganded HSV-2 protease structure) as defined by position in Figure 1 herein [SEQ ID NO: 4].

Also provided is a novel HSV-1 protease composition characterized by a three dimensional active catalytic site of three conserved amino acid residues, Ser 129, His 61, His 148, four additional amino acid residues Ala 131, Cys 152, Arg 156, and Arg 157, as defined by position in Figure 1 herein [SEQ ID NO: 3].

In yet another aspect, the present invention provides a novel CMV protease composition characterized by a three dimensional active catalytic site of six conserved amino acid residues: Ser 132, His 63, His 157, Asp 65, Cys 161 and Ser 134. Additionally, the CMV catalytic site may also contain either or both Arg 165 and Arg 166, as defined by their position in Figure 1 herein [SEQ ID NO: 1]. The CMV structure further reveals a novel active site tetrad, formed by

Ser132-His63-His157-Asp65 [SEQ ID NO: 1]. In still another aspect, the present invention provides a novel CMV protease composition characterized by a three dimensional active catalytic site of six conserved amino acid residues, Ser 132, His 63, His 157, Cys 161, Arg 165, and Arg 166 and three non-conserved amino acid residues Ser 134, Asp 65, and Asn 60, as defined by position in Figure 1 herein [SEQ ID NO: 1].

The invention further provides a novel VZV protease composition characterized by a three dimensional active catalytic site of three conserved amino acid residues, Ser 120, His 52, His 139, and five additional amino acid residues Ser 122, Cys 143, Arg 147, Arg 148 and Lys 54, as defined by the amino acid positions in Fig. 1 [SEQ ID NO: 5].

I. The Novel Protease Crystalline Three-Dimensional Structure

The present invention provides novel protease crystalline structures based on the herpes proteases. The three dimensional (3D) structure of the HSV-1, HSV-2, CMV and VZV proteases provided herein reveal a unique fold that has not been reported for any serine protease, and a novel active site consisting of a novel catalytic triad formed by 3D interactions of the amino acids Ser, His and His. An unusual dimer interface that is important to protease activity was also found in the crystals for each of these proteases. In yet another aspect, the present invention provides for a novel herpes protease composition characterized by a dimer interface of two herpes protease molecules. Inhibition of this dimer interface by inhibitors which perturb interaction with these dimer interfaces. Inhibitors that perturb or interact with these dimer interfaces are yet another therapeutic target for the design and selection of therapeutic agents against herpes proteases.

Listed in Fig. 1 are known amino acid sequences for the herpes family proteases HHV-6, HSV-1, HSV-2, VZV, EBV and CMV, aligned to illustrate the homologies between them [SEQ ID NO: 1-6]. As seen in Fig. 1, when compared to members of the alpha subfamily, HSV-2, HSV-1, and VZV protease amino acid sequences are rather conserved (HSV-1 protease is 50% identical to VZV protease and 90% identical to HSV-2 protease; VZV protease is 26% identical to CMV protease); CMV protease differs in having a shorter N-terminus and two multi-residue insertions (at CMV protease amino acid residues 40-47 and 147-152, SEQ ID NO: 1).

According to the present invention, the crystal structure of human HSV-1, liganded and unliganded HSV-2, CMV and VZV proteases have been determined. These protease crystal structures reveal a fold and an active site that are distinct from other known, non-herpes serine proteases. Details of structure determination and refinement are presented in Figures 2 - 26 below.

Further refinement of the atomic coordinates will change the numbers in Figures 2 - 26, refinement of the crystal structure from another crystal form will result in a new set of coordinates, determination of the crystal structure of another herpes protease will also result in a different set of numbers for coordinates in these figures. However, distances and angles will remain the same within experimental error, and relative conformation of residues in the active site will remain the same within experimental error. Also for example, the amino acid sequence of the herpes proteases can be varied by mutation derivatization or by use of a different source of the protein, as described herein.

A. HSV-1 and HSV-2

The crystal structures of HSV-1 and HSV-2 have been determined, as described herein, and are discussed in tandem below.

The crystal structure of human HSV-1 protease has been determined at 3.5 Å resolution. The structure was determined using the method of molecular replacement (MR) and refined to an R-factor of 36.9% (10.0-3.5 Å, using $|F_o| > 2\sigma$ $|F_o|$ data).

The crystal structures of human DIP-liganded HSV-2 protease and the unliganded HSV-2 protease have been determined at 2.5 Å and 2.8 Å resolution, respectively. The DIP-liganded HSV-2 protease structure was determined using the methods of multiple isomorphous replacement (MIR) and MR and refined to an R-factor of 20.5% (10.0-2.5 Å, using $|F_o| > 2\sigma$ $|F_o|$ data) with root-mean-square deviations on bond lengths and bond angles of 0.016 Å and 1.9°, respectively. The unliganded structure was determined using difference Fourier methods using the DIP-liganded HSV-2 protease structure and refined to an R factor of 22.4 %. The root-mean-square deviations of bond lengths and bond angles are 0.017 Å and 2.1 Å.

Although human HSV-1 and HSV-2 proteases contain 247 amino acids, the models of these proteases are represented by 214 residues for HSV-1 protease and 217 residues for DIP-liganded HSV-2 protease. With respect to HSV-1 protease, residues 1-14 and residues in two surface loops 102-110, and 134-143 are disordered in the crystal [SEQ ID NO: 3]. With respect to HSV-2, residues 1-16 and residues in two surface loops 104-110, and 134-140 are disordered in the crystal [SEQ ID NO: 4]. The model of unliganded HSV-2 protease has 215 residues where 1-16, 104-112, and 134-140 are disordered in the crystal [SEQ ID NO: 4].

The fold in each of the HSV-1 and HSV-2 proteases is characterized by 7 b-strands and 7 a-helices as depicted in Figures 1, 29, and 30. As discussed herein, the loop containing residues 25-55 in the CMV protease [SEQ ID NO: 1] is disordered in the crystal, but the corresponding loop in the HSV-1 and HSV-2 protease crystals are observed.

Fig. 2A-2F disclose the coordinates of the residues of the novel HSV-2 catalytic triad and other residues and water molecules within 5.5 Å of the DIP modified Ser 129 (including the DIP ligand) in the active site. These include amino acid residues Ser 129, His 61, His 148, Ser 131, Cys 152, Arg 156, Arg 157, Leu 27, Val 128, Leu 130, and, water molecules Wat1 and Wat2 of the DIP-liganded HSV-2 protease [SEQ ID NO: 4] according to this invention. Fig. 3A-3E disclose the coordinates of residues of the novel catalytic triad and other residues in the active site of the unliganded HSV-2 protease. These include residues Ser 129, His 61, His 148, Ser 131, Cys 152, Arg 156, Arg 157, Leu 27, Val 128, and Leu 130. These data are reported for crystals with lattice constants of $A=71.7$ Å, $B=87.4$ Å, $C=77.3$ Å, $\alpha=90^\circ$, $\beta=90^\circ$ and $\gamma=90^\circ$, with a space group = $P2_12_12$. The liganded and unliganded crystal forms have the same cell dimensions and space group. The data is reported in Protein Data Bank (PDB) format, illustrating the atom, i.e., nitrogen, oxygen, carbon (at α , β , δ or γ positions in the atom); the amino acid residue in which the atom is located with amino acid number, and the coordinates X, Y and Z in Angstroms (Å) within the crystal lattice. Also illustrated is the occupancy of the atom, noting that each atom in the active site has a unique position in the crystal. The data also report the B or Temperature Factor, which indicates the degree of thermal motion of the atom in volume measurements (Å²). Figures 4A-4MMM and 5A-5DDD disclose the protein coordinates of the DIP-liganded HSV-2 and unliganded protease crystalline structure of the invention respectively, including the active site.

Figure 6A-6B disclose the coordinates of residues in the active site region (at amino acid residues Ser 129, His 61, His 148, Ala 131, Cys 152, Arg 156, Arg 157) of the HSV-1 protease [SEQ ID NO: 3] according to this invention. These data are reported for crystals with lattice constants of $a=79.62$ Å, $b=81.18$ Å, $c=93.36$ Å, $\alpha=115.49^\circ$, $\beta=98.36^\circ$ and $\gamma=109.18^\circ$, with a space group = $P1$. The data is reported as described above for HSV-2 protease. Figure 7A-7DDD illustrate the orthogonal three dimensional coordinates in Angstroms and B factors for HSV1 protease.

Figure 8A-8X provide the distances (in Angstroms) between any protein residue that has an atom within a 5.5 Å radius of any atom of Ser 129 [SEQ ID NO: 4] covalently bonded to DIP in the DIP-liganded HSV-2 protease structure. Figure 9A-9I provide distances (in Angstroms) between every two atoms that are within 5.0 Å of the active site residues of the unliganded HSV-2 protease. The atoms are indicated in this figure by the amino acid position number in which the atom appears, followed by the atom designation, i.e., nitrogen, oxygen, etc. as described for Figures 2 and 3.

Figure 10A-10B provide the distances (in Angstroms) between every two atoms that are less than 5 Å from the active site of HSV-1 protease. The atoms are indicated as described above for HSV-2 protease. Figure 11A-11LLL provide the bond angles (in degrees) between any atom of HSV-2/DIP-modified Ser 129 and any two protein residue atoms that are within a 5.5 Å radius of the DIP modified Ser 129 (Overall Active Site Residues Only). Figure 12A-12Q provide the bond angles (in degrees) between interresidue atoms that are within 5 Å apart in the active site region near Ser 129, His 61 and His 148 [SEQ ID NO: 4] of the unliganded HSV-2 protease. Figure 13A-13D provide the bond angles between interresidue atoms that are within 5 Å apart in the active site region near Ser 129, His 61 and His 148 of the HSV-1 protease [SEQ ID NO: 3] of this invention. Figures 14 and 15 provide the dihedral angles of the active site formed by Ser 129, His 61 and His 148 [SEQ ID NO: 4] of the protease, for the DIP-liganded HSV-2 and unliganded proteases, respectively. Figure 16 provides the dihedral angles of the active site formed by Ser 129, His 61 and His 148 of the HSV-1 protease [SEQ ID NO: 3].

The novel folds of the HSV-2 and HSV-1 protease crystal structures are discussed in part D. below; the novel active sites are discussed in part E.

B. CMV Protease

The crystal structure of human CMV protease has been determined at 2.5 Å resolution. As described in more detail in Example 3 below, a CMV protease sequence (CMV A143V) was employed in which the alanine residue at position 143 was replaced by a valine. This mutation had no effect on the enzyme activity, but was necessary to eliminate the nick after Ala 143 seen in preparations of the native enzyme [Welch I, and Baum *et al.*, cited above]. The structure was determined using MIR, and refined to an R-factor of 18.5% (7.0-2.5 Å, using $|Fo| > 1\sigma$ $|Fo|$ data) with root-mean-square deviations on bond lengths and bond angles of 0.017 Å and 2.2°, respectively.

Although human CMV protease contains 256 amino acids, the model of the enzyme provided herein is represented by 202 residues. Residues 1-8 and residues in three surface loops (residues 25-55, 143-153 and 205-208 of SEQ ID NO: 1) are found disordered and are not present in Figure 17A-17E. Details of structure determination and refinement are presented in Figures 17 through 21.

Figure 17A-17E disclose the protein coordinates near the active site region (at amino acid residues Ser132, His63, Ser 134, Cys161, Arg165 and His157, and including Arg166 of SEQ ID NO: 1) of the CMV protease according to this invention. These data are reported for crystal lattice constants of $a=58.7$ Å, $b=58.7$ Å, $c=131.0$ Å, $\alpha=90^\circ$, $\beta=90^\circ$ and $\gamma=90^\circ$, with a space group = $P4_322$. The data is reported in Protein Data Bank (PDB) format, as described above for HSV-2 and HSV-1. Figure 18A-18C provide the distances in Angstroms between every two atoms that are less than 5 Å from the active site for CMV protease. Figure 19A-19D illustrate the bond angles between interresidue atoms that are within four Å apart in the active site region near Ser132, His63, His157 and Asp65 of the CMV protease [SEQ ID NO: 1] according to this invention. Figure 20 provides the dihedral angles of the tetrad active site formed by Ser132, His63,

His157 and Asp65 of the protease [SEQ ID NO: 1]. Figure 21A-21DD disclose the protein coordinates of the CMV protease crystalline structure of the invention, including the active site. See D. below for discussion of the CMV crystal structure folds and part E. for further discussion of the active site.

5 C. VZV Protease

The crystal structure of human VZV protease has been determined at 3.0 Å resolution. As described in more detail in the Example 6 below, a VZV protease sequence was employed in which the mutant has the N-terminal nine (9) amino acids deleted. This mutation had little effect on the enzyme activity. The structure was determined using the methods of MR and single isomorphous replacement (SIR) and refined to an R-factor of 22.3% (7.0-3.0 Å, using $|F_o| > 1\sigma |F_o|$ data) with root-mean-square deviations on bond lengths and bond angles of 0.014 Å and 2.1°, respectively.

The model of the VZV enzyme used in the crystal structure study consisted of residues 11-236 of SEQ ID NO: 5. The VZV structure model consists of 211 amino acids. A surface loop of aa 127-136 is disordered in the crystal, as are the last 5 amino acids at the C-terminal of VZV. In VZV, an additional helix has been observed in the region between residues 31-39 of SEQ ID NO: 5. The fold is characterized by 7β strand and 8 α-helices as depicted in Figs. 1 and 35. The loop containing residues 22-55 in the CMV protease is disordered in the crystal, but as for HSV-1 and HSV-2 proteases, the corresponding loop in the VZV protease crystal is observed. This loop is situated near the active site and is proposed to enclose part of the substrate binding groove, the S subsites [I. Schechter and A. Berger, *Biochem. Biophys. Res. Commun.*, 27:157-162, (1967)].

Fig. 22A-22C disclose only the protein coordinates near the active site region (at amino acid residues Ser 120, Ser 122, His 52, Lys 54, Cys 143, Arg 147 and Arg 148 of SEQ ID NO: 5) of the VZV protease according to this invention. These data are reported for crystals with lattice constants of $a=90.0$ Å, $b=90.0$ Å, $c=117.4$ Å, $\alpha=90^\circ$, $\beta=90^\circ$ and $\gamma=90^\circ$, with a space group = $P6_422$. Fig. 23A-23SS disclose protein coordinates of the VZV protease crystalline structure. Fig. 24A-24C provide the distances in Angstroms between every two atoms that are less than 5Å from the active site for VZV protease. Fig. 25A-25D illustrate the bond angles between interresidue atoms that are within four Å apart in the active site region near Ser 120, His 52 and His 139 of the VZV protease [SEQ ID NO: 5] according to this invention. Fig. 26 provides the dihedral angles of the tetrad active site formed by Ser 120, His 52 and His 139 of the protease [SEQ ID NO: 5].

The VZV protease crystal structure novel fold is discussed in more detail in D. below. The Novel active site is discussed in part E.

D. The novel fold

1. HSV-2 and HSV-1 Proteases

With reference to Figures 27A, B and C, the structures of the liganded and unliganded forms of HSV-2 are nearly identical. The binding of DIP to the HSV-2 protease structure does not alter the conformation of the enzyme. The root mean square deviation between the liganded and unliganded forms is 0.4 Å. The presence of the DIP changes interactions only within the active site of the enzyme but not the location of the active site or overall three dimensional structure of the enzyme.

The overall folds of the HSV-1 and HSV-2 protease dimers are comprised of two β-barrels. The folds of the HSV-2 protease are discussed above. The overall fold of the HSV-1 protease dimer is illustrated in Figs. 28A and 28B. For each protease, seven b-strands form the core of each barrel (Fig 29A,B,C for HSV-2 and 30A, 30B for HSV-1), each of which can be classified as an orthogonally packed β-barrel [(Chothia and Janin *Biochemistry*, 21: 3955-3965 (1982)), with the following exceptions: strands B6 and B7 are parallel, unlike most orthogonally packed β-barrels. Also, strand B3 (aa 65-77) is a β-bend that closes one corner of the barrel, but the other corner lacks this kind of classical closure and is maintained by only two hydrogen bonds between strand B5 (aa 127-133) and B7 (aa 161-166) [SEQ ID NO: 3 and 4]. Among well known serine proteases, the N-terminal domain of trypsin is also an orthogonally packed β-barrel, but superposition with the HSV-1 or HSV-2 protease barrel does not reveal any similarities and positions the active sites in different regions of the fold. Moreover, the β-strands (Fig. 31 for HSV-2 and HSV-1) are arranged differently in the two structures. For example, the first four strands of HSV-2 protease (B1, B2, B3 and B4) form a typical Greek Key motif while those in trypsin do not. Therefore, it is reasonable to conclude that the HSV-2 and HSV-1 protease barrels are evolutionally unrelated to other known non-herpes serine proteases.

The seven alpha helices of liganded and unliganded HSV-2 protease and HSV-1 do not surround the barrel but rather cluster towards the ends. Alpha helix A1 seals one end while helices A2, A3, A6, and A7 close the other. Of these, helices A6 and A2 with the corresponding helices of the dimer mate define a unique dimer interface that reveals an approximately 30 degree twist between the corresponding monomers. While four of the seven helices are at either end of the barrel the other two are on the same side of the structure, away from the active site.

For the DIP-liganded HSV-2 protease structure, the transition state analog inhibitor diisopropyl fluorophosphate

was added to the enzyme in which the highly reactive (P-F) linkage undergoes displacement by the serine hydroxyl group. Once bound to the nucleophile, (enzyme) the ligand is referred to as diisopropyl phosphate. The DIP-liganded HSV-2 protease has the inhibitor diisopropyl phosphate covalently bound to the active site serine (Ser 129).

Unlike trypsin, the active sites of HSV-1 and HSV-2 proteases do not lie at the intersection of the two domains but rather bind in a cleft formed by one side of the barrel at strand B5 and a small loop between strands B6 and B7 made of residues 153-157 (Figs. 27A,B,C and 29A,B,C for HSV-2 and Figs. 28A, 28B and 30A, 30B for HSV-1). The DIP C_β atom of the DIP-liganded HSV-2 protease is 17 Å from the closest point between the two monomers at helix A6. In each of the HSV-1 and HSV-2 protease structures, residues 34-38 [SEQ ID NO: 3 and 4] in the large loop between B1 and A1 approach the top of the cleft but do not completely cover it. The loop of residues 134-140 [SEQ ID NO: 3 and 4] is disordered in the HSV-1 and HSV-2 structures. This loop is a region of low homology among the herpes proteases (Fig 1); and may suggest different conformations of the loop. Residues 104-110 and 104-112 are disordered in the DIP-liganded HSV-2 and unliganded HSV-2 protease structures, respectively [SEQ ID NO: 4]. Residues 102-110 of HSV-1 [SEQ ID NO: 3] are disordered in the structure. These regions represent regions of low homology among the herpes proteases; however, the corresponding regions are ordered in both the VZV and CMV proteases, where a small alpha helix is seen.

An intriguing non-crystallographic dimer interface in each of the HSV-1 and HSV-2 proteases is made up of the interactions between helices A6 and A2 with the corresponding helices in the dimer mate. The dimer interface is identical between the liganded and unliganded HSV-2 proteases. These same helices also interact in CMV but with a different orientation in relation to each other. In CMV protease the two A6 helices of each monomer are nearly co-axial. In the HSV-1 and HSV-2 proteases they are separated at the N-terminal ends by about 30 degrees, at a distance of nearly 14 Å. Because of the twist between the A6 helices in the HSV-1 and HSV-2 proteases, contacts can only be formed between the C-terminal ends of the helices. In both the liganded and unliganded HSV-2 proteases, a hydrogen bond (3.0 Å) is seen between the side chains of His 211 and Glu 207 [SEQ ID NO: 4]. When comparing the dimer interface of HSV-1, HSV-2 and CMV proteases, changes are also seen in the A2 helix position with respect to A6. In HSV-2 protease [SEQ ID NO: 4], hydrogen bonds are formed between Ala 98 on A2 to both Ser 215-OH (2.7 Å) and Asn 219 (3.3 Å) on A6. These two interactions and that between 211 and 207 [SEQ ID NO: 4] do not occur in either CMV or VZV proteases. In CMV and VZV proteases the dimer interface is along a two-fold crystallographic axis, which could cause subtle changes in the interactions between the monomers.

There are other notable structural differences between HSV-2 and HSV-1 and those of the CMV and VZV proteases discussed below. One difference is in the segment between A2 and A3. In the structure of CMV protease, this segment assumed a "closed" conformation, making intra-molecular contacts and being part of the dimer interface. In the VZV protease structure, this segment adapts a completely "open" conformation, interacting only with another symmetry-related molecule to form a different dimer interface. In the liganded and unliganded HSV-2 protease structures, part of this loop is disordered but is a close distance (9 Å) to another symmetry-related molecule. This suggests that HSV-2 and VZV proteases may be capable of using this segment to form higher order oligomers.

It has been reported that CMV protease dimerization is important for maintaining the activity of the protease [Darke, et al., *J. Biol. Chem.*, 271, pp. 7445-7449 (1996)]. In fact, the Darke publication and S. Margosiak, et al. *Biochemistry* 35, 5300-5307 (1996) have shown that the CMV protease molecules self-associate to form dimers in solution with a monomer-dimer equilibrium constant of approximately 10^{-6} M and that the dimeric form of the protease is the only active species. There is now a similar report on the dimer formation of HSV-1 protease [Schmidt, U. and Darke, P. L., *J. Biol. Chem.*, 272, pp. 7732-7735 (1997)], but with a similar dimerization response in the presence of glycerol [Darke et al., *J. Biol. Chem.*, 270: 22697-22700 (1995)]. Furthermore, enzymatic assays are often reported in the presence of aggregation-promoting reagents such as glycerol or citrates [Burck et al., Hall et al., both cited above].

Based on the present structure it is difficult to determine why the dimer is required for activity, since the interface is not near either active site. The addition of the covalent inhibitor DIP does not appear to alter the dimer interface. However, rearrangements of the helices at the interface in the absence of a dimer could have profound effects on the conformation in the active site region. Thus, dimerization is believed to stabilize the conformation of helix A6.

2. The CMV and VZV Proteases

Unlike the structures of other serine proteases having two distinct β -barrel domains, the structures of each of the herpes proteases herein have a single domain.

The overall fold of the CMV and VZV monomers can be best described as a 7-stranded β -barrel core which in CMV is decorated with seven α -helices on three sides (see Figs. 32A and 32B) and in VZV is decorated with eight α -helices (Figs. 33A and 33B). The core β -barrel can be classified as an orthogonal packed β -barrel as described in detail by C. Chothia & J. Janin, *Biochemistry*, 21: 3955-3965 (1982). Of the seven helices of CMV, three were found between strand β 4 and β 5, and four helices after strand β 7 (Fig. 34).

Certain features of the CMV protease and VZV protease barrels are quite distinct. First, the CMV protease and VZV protease barrels contain two parallel strands (Figs. 34 and 35) and thus are mixed β -barrels, while most of the

orthogonal packed β -barrels are formed exclusively from anti-parallel strands. Second, strand $\beta 3$ [aa67-78 of CMV (SEQ ID NO: 1) and aa57-67 of VZV (SEQ ID NO: 5)] are β -bends that close one corner of the barrel, but the other corner lacks this kind of classical closure and is maintained by only two hydrogen bonds between strand B5 [aa130-135 of CMV (SEQ ID NO: 1) and aa118-123 of VZV (SEQ ID NO: 5)] and B7 [aa169-175 of CMV (SEQ ID NO: 1) and aa151-157 of VZV (SEQ ID NO: 5)].

Interestingly, the N-terminal β -barrel of trypsin's prototype serine protease is an anti-parallel β -barrel that is also orthogonally packed. However, superposition of the CMV protease, VZV protease and trypsin barrels did not reveal any further resemblance, and show the enzyme active sites of the CMV and VZV proteases are at completely different regions of the fold than the active site of trypsin. Moreover, the CMV and VZV β -strands (Fig. 34 and Fig. 35) are arranged differently than in trypsin. For example, the first four strands of CMV and VZV proteases (B1, B2, B3 and B4) form a typical Greek Key motif, while those in trypsin do not. Therefore, it is reasonable to conclude that the CMV protease and VZV protease barrels are evolutionally unrelated to other, non-herpes serine proteases. The overall fold is also unique to CMV, VZV and other herpes proteases.

An intriguing dimer interface in CMV and VZV proteases has been identified around two-fold crystallographic axes (Figs. 36A and 36B, 37). The dimer interface is mainly made-up of a set of four helices (A1, A2, A3 and A6) of one monomer that surrounds helix A6 of the other monomer, where the two symmetry-related A6 helices are parallel (Fig. 37). The dimer interface is predominantly hydrophobic, involving many side chain van der Waals interactions for residues such as phenylalanines, leucines and valines. Despite the tight packing in the crystal, this dimer interface is much more significant than that of other inter-molecular interfaces within the crystal. The arrangements of the helices and the extent of the interface seem to suggest that this is not a simple coincidence of crystal packing.

The dimer interface is of importance in maintaining the activity of the proteases. The calculated interface area is between 850 (Connolly) to 1300 \AA^2 (GRASP) from the crystal structures of CMV and VZV proteases. As for HSV-2 and HSV-1, from the crystal structures, it is noted that the dimer interface is not in the immediate vicinity of the active site. Also, the active sites of the two monomers are quite distant from each other (Fig. 36B and Fig. 37).

Although the dimer interfaces in VZV and CMV proteases are similar, there are notable differences in their structures. Helices A6 from both monomers were almost parallel in the structure of CMV protease, but helix A6 is twisted about 30° in the VZV protease structure (Fig. 37). The helix A6 in VZV protease has one more turn at the N-terminal, and the loops connecting A5 and A6 are quite different in the two structures (Fig. 1). The biggest difference resides in the segment containing the small helix A2. In the structure of CMV protease, this segment assumed a "closed" conformation, making intra-molecular contacts and being part of the dimer interface. However, in the VZV protease structure, this segment adapts a completely "open" conformation, interacting only with another symmetry-related molecule to form a different dimer interface (Fig. 37). This suggests that VZV protease may be capable of using this segment to form higher order oligomers. By analogy with CMV protease, the VZV protease dimer is essential for enhanced catalytic activity. In the absence of a dimer, the rearrangements of helices involved in the interface may have profound effects on the conformation in the active site region. For example, the A6 helix may move toward the active site cavity and therefore affect the positioning of residues in the active site or it may simply block access to the substrate.

E. The novel active site

The catalytic mechanism of classical serine proteases involves an active site triad composed of a serine, histidine and an aspartic acid. However, although several prior art studies focused on mutagenesis of aspartic and glutamic acids of herpes proteases, none led to a correct identification of the third member of the herpes protease catalytic triad.

The crystal structure of liganded and unliganded HSV-2 protease reveals an active site composed of a serine (Ser 129), a histidine (His 61), and a third residue also a histidine (His 148) (Fig 38A,B), sequences which are conserved in all known herpes proteases (Fig. 1). The crystal structure of HSV-1 protease reveals an identical active site (Fig. 39A). The crystal structure is in agreement with early protease inhibition experiments on HSV-1 protease (sharing 90% sequence identity and identical numbering to HSV-2 protease) that identified HSV-1 as a serine protease and that substitution of His 148 and His 61 abolished [SEQ ID NO: 3] enzymatic activity (Liu & Roizman, Dilanni I). Similar studies on CMV protease had also demonstrated the homologous residues to His 61 and Ser 129 to be essential (Stevens, Welch I). Although several studies focused on mutagenesis of aspartic and glutamic acids of herpes proteases, none led to a correct identification of the third member of the catalytic triad. Figure 38A shows the DIP molecule covalently bound to Ser 129 [SEQ ID NO: 4]. This is consistent with mutagenesis and chemical modification studies that identified Ser 129 as the active site nucleophile in HSV-1 protease [SEQ ID NO: 3] (Dilanni II).

As with HSV-2 and HSV-1 proteases, the crystal structure of the CMV and VZV proteases of the invention reveals a novel active site containing a serine [Ser 132 for CMV (SEQ ID NO: 1) and Ser 120 for VZV (SEQ ID NO: 5)] and a histidine [His 63 for CMV (SEQ ID NO: 1) and His 52 for VZV (SEQ ID NO: 5)], with the third member of the catalytic triad being a histidine [His 157 for CMV (SEQ ID NO: 1) and His 139 for VZV (SEQ ID NO: 5)] instead of aspartic acid. Mutagenesis and chemical modification studies had identified Ser 132/Ser120 [SEQ ID NO: 1 and 5, respectively] and His 63/His52 [SEQ ID NO: 1 and 5, respectively] as part of the catalytic triad [Welch I, Stevens *et al.*, cited above]. Both

residues are absolutely conserved in all herpes proteases (Fig. 1).

1. HSV-2 and HSV-1 Proteases

The active site of DIP-liganded HSV-2 protease shows a network of hydrogen bonding between the enzyme active site, the ligand, and two central water molecules (Wat1 and Wat2 (Fig. 38A)). The crucial elements of the HSV-1 and HSV-2 active sites are strikingly similar to trypsin even though the two HSV enzymes share little sequence homology with trypsin and the overall tertiary structures are completely different to trypsin. An overlay of the catalytic triad of γ -chymotrypsin bound to mono-isopropyl phosphate (MIP) with that of the DIP-liganded HSV-2 structure (Fig. 38C), and an overlay of the catalytic triad of trypsin (BPD code 1SGT) with that of the HSV-1 protease structure shows this similarity (Fig. 39B). In Fig. 38C, significant overlap is seen between the peptide backbone stabilizing the P=O oxygen of DIP, the catalytic serine residues, and His 61 and His 57 side chains of γ -chymotrypsin and DIP-liganded HSV-2 protease, respectively. Figure 38C also reveals the overlap of Asp 102 and His 148 [SEQ ID NO: 4], supporting the role of this histidine in catalysis, despite its apparent lack of hydrogen bonds in this structure. Similar results are revealed in Fig. 39B. Not only does this confirm the role of His 148 [SEQ ID NO: 3 and 4] in catalysis, but it also suggests the possibility of converting the HSV-2 and HSV-1 enzymes into those having a normal catalytic triad by replacing His 148 [SEQ ID NO: 3 and 4] with an aspartic acid.

Because of the presence of the covalently bound inhibitor DIP, His 61 does not appear to hydrogen bond to Ser 129 [SEQ ID NO: 4] but instead maintains a close interaction with Ser 131 (2.5 Å). This can be compared to a slightly different hydrogen bonding network in apo CMV protease (Fig. 38D) where His 61 has hydrogen bonds to both Ser 129 and His 148 and Ser 131 clearly interacts with His 148 [SEQ ID NO: 1]. This is similar to the hydrogen bonding network in the γ -chymotrypsin/MIP structure where Ser 214 maintains a close hydrogen bond to Asp 102 (Fig. 38C) [SEQ ID NO: 3]. Despite its location in the active site, Ser 131 has been found to be nonessential for catalysis in CMV protease [SEQ ID NO: 1] (Welch I). This position is also an Ala residue in HSV-1 (Fig. 1). The average B factor of the side chain atoms of His 61 in the DIP-liganded HSV-2 protease [SEQ ID NO: 4] is 51 Å², more than twice the average B-factor of the structure, indicating that it is mobile. A rotation about the C β -C γ bond could allow a hydrogen bond to Ser 129, and a subsequent rotation about the same bond in His 148 could allow a hydrogen bond between these two residues. These two rotations would present a hydrogen bond of 3.0 Å between His 148 and His 61, about the same distance as in the uncomplexed CMV structure, and thus an alternative set of hydrogen bonds.

The active site of HSV-1 protease is very similar to that of HSV-2 protease with some minor differences (Fig. 39C). These differences are most likely because the HSV-2 protease had a covalently bound DIP inhibitor (not shown in the figure, for clarity) bound to the Ser 129 which prevented a hydrogen bond between Ser 129 and His 61 [SEQ ID NO: 4]. This hydrogen bond is present in the HSV-1 protease structure in which the imidazole ring has turned by about 90° to accommodate this hydrogen bond. Also, position 131 is an Alanine in HSV-1 protease [SEQ ID NO: 3] and thus cannot maintain any hydrogen bonds to either His 61 or His 148 as has been seen in HSV-2 [SEQ ID NO: 4] and the other herpes proteases. There is a slightly different hydrogen bonding network in the unliganded (or apo) CMV protease structure (Fig. 39D) where the equivalent residue of His 61 has hydrogen bonds to both Ser 129 and His 148 and Ser 131 clearly interacts with His 148 [SEQ ID NO: 1].

Another absolutely conserved residue in both HSV-1 and HSV-2 is Cys 152 [SEQ ID NO: 4] which is within the vicinity of the active site. It is also conserved and in an identical position in trypsin. However, it has limited contact with the DIP ligand (Fig. 38A): the C152 C γ atom maintains a van der Waals contact (3.8 Å) to a Ser 129 methyl group. Thus, it is difficult to imagine it being a suitable proton acceptor because of its nature and position. Also, this cysteine is not essential for catalytic activity in HSV-1 protease (Liu & Roizman III), or CMV protease (Welch I).

An oxyanion hole for DIP-liganded HSV-2 protease can be identified in the present invention. Such an oxyanion hole for HSV-1 protease can also be identified based on its nearly identical structure to the HSV-2 proteases (Fig. 39C). An oxyanion hole is that portion of the protease which provides an environment for the stabilization of the tetrahedral intermediate. In DIP-liganded HSV-2 protease, the amide nitrogen of Arg 156 and Wat1 stabilize the P=O oxygen of the DIP and define the oxyanion hole of the enzyme (Fig. 38A). Wat1 is stabilized by hydrogen bonds to Wat2 (2.7 Å) and Val128 (2.8 Å). Correspondingly, Wat 2 is held by hydrogen bonds to backbone atoms of Leu 130 (2.9 Å) and Leu127 (2.9 Å) and Arg 157N ϵ (3.2 Å). The alignment with CMV protease (Fig. 38D) also shows a single water molecule in the active site region of this enzyme, closely overlapping with Wat2 in the HSV-2 protease structure. This water molecule maintains the same protein backbone hydrogen bonds as does Wat2 in HSV-2 and could help hold the side chain of Arg 157 in place. In HSV-1 protease, the backbone atoms at Arg156 are the same as in DIP-liganded HSV-2 protease, making it likely this residue also helps define the oxyanion hole in HSV-1 protease. Arg156 and Arg 157 are absolutely conserved in all herpes proteases and present an overall positive charge near the oxyanion hole. The stability of this region is reflected here where Arg 157 makes two hydrogen bonds to backbone atoms of Leu 130 and Leu 38 both absolutely conserved in all herpes proteases (Fig. 1). The alignment with γ -chymotrypsin shows how close the P=O oxygen of MIP is stabilized by a hydrogen bond to the amide nitrogen of Gly 193. In DIP-liganded HSV-2 protease, the amide nitrogen of Arg 156 closely corresponds to that of Gly 193 even though the overall structure of the two enzymes

is completely different (Fig. 38C).

The active site of liganded and unliganded human HSV-2 protease and HSV-1 protease sit at a very shallow and mostly exposed region of the protease (Figs. 27A,B,C; 29A,B,C; Fig. 28A, 28B, 30A, 30B). Shallowness of the active site cavity is not really surprising given that the scissile bond (the bond which gets cleaved) recognized by all herpes proteases is between two small amino acid residues (Ala-Ser). Missing around the active site cavity are amino acid residues 134-140 [SEQ ID NO: 3 and 4], that are part of a surface loop. Interestingly, a mutant with a five residue deletion in the corresponding loop in CMV protease residue was shown to be fully active, but with altered substrate specificity [Welch I, cited above]. Given this loop's proximity to the active site cavity, it may be a flexible flap that is involved in substrate recognition.

Since the CMV protease structure misses two large loops near the active site, it was difficult to speculate about the substrate binding mode of the enzyme. With the liganded and unliganded HSV-2 protease and HSV-1 protease structures, the missing loop containing residues 32-54 [SEQ ID NO: 3 and 4] becomes ordered, possibly having a role in substrate recognition (Fig. 27A, Fig. 28A). There are two grooves, or depressions near the active site. One of the grooves is deep and wide, found in a region that is reminiscent of the S' subsites of classical serine proteases. One side of the groove is delineated by the active site residues while the other is formed by a side of helix A6, a critical structural feature of the enzyme. The other groove is relatively narrow and is formed by B5, including the catalytic triad, on one side and the other made by the small loop of 154-160 [SEQ ID NO: 3 and 4] which includes the conserved GRR sequence (Fig. 1). This region is also in a position that is not very different from the unprimed (S) subsites in classical serine proteases. The substrate peptide (at least P2-P4) could be inserted into the groove with its main chain forming an antiparallel β -sheet with strand B5 and B6. Of course, structural studies of enzyme-substrate analog complexes are needed for proving this model.

2. CMV Protease and VZV Protease Active Sites

None of the aspartic or glutamic acids is absolutely conserved in all herpes proteases. Glu 122 was proposed as a member of the catalytic triad [Cox *et al.*, cited above] for CMV protease. However, it is found to be distant from the catalytic site in the CMV protease crystal structure. This glutamic acid is buried near the C-terminus of the protein, making a salt bridge with Lys 255 of CMV protease (Glu 122 OE1-Lys 255 NZ, 2.7 Å) and a hydrogen bond with the backbone nitrogen of Asp 118 of CMV protease (Glu122 OE2-Asp 118 N, 3.1 Å) [SEQ ID NO: 1]. Therefore, its importance to the protease can only be attributed to its role in maintaining the overall structure of the protease, rather than being directly involved in the catalytic machinery.

Although His 157 (for CMV, SEQ ID NO: 1) and His 139 (for VZV, SEQ ID NO: 5) are absolutely conserved among all herpes proteases, and mutagenesis of this histidine was shown to abolish enzymatic activity in HSV-1 [Liu II, cited above] and CMV proteases in HSV-1 [Welch I, cited above], no one has suggested that it has a role as the third member of the catalytic triad. Abolition of enzymatic activity does not necessarily necessitate involvement in catalytic activity but could be a result of changes in protein conformation.

As expected, the O γ atom of Ser 132 for CMV protease [SEQ ID NO: 1] (Ser 120 for VZV protease [SEQ ID NO: 5]) is found to be in the vicinity of His 63 for CMV protease (His52 for VZV protease), with a distance of 3.3 Å from its N ϵ 2 nitrogen for CMV protease (3.6 Å for VZV protease). Given the presence of about 0.4 Å coordinates error and the absence of a substrate in the active site, the 3.3 Å distance for CMV (3.6 Å for VZV) does not preclude these two residues from being the catalytic residues. Surprisingly, the conserved second histidine (His 157 for CMV protease [SEQ ID NO: 1] and His 139 for VZV protease [SEQ ID NO: 5]) is hydrogen bonded to the side chain of His 63 (His 63 N δ 1-His 157 N ϵ 2, 3.2 Å) for CMV protease and His 52 (His 52 N δ 1-His 139 N ϵ 2, 3.2 Å) for VZV protease, making it the third member of the catalytic triad. In CMV protease [SEQ ID NO: 1], the only acidic residue in the vicinity is Asp 65, with its O δ 1 atom 3.9 Å away from the N δ 1 nitrogen of His 157. In VZV protease [SEQ ID NO: 5], a basic residue Lys 54 replaces the Asp 65 of CMV protease, with its O δ 1 atom 5.1 Å away from the N ϵ 2 nitrogen of His 139, too far to influence catalysis in VZV protease.

In the CMV protease crystal structure, Asp 65 forms a salt-bridge with Arg 109 of a neighboring, symmetry-related molecule other than the aforementioned dimer (Asp 65 O δ 2-Arg 109 NH1, 2.8 Å). Therefore, in the absence of this salt-bridge in solution, Asp 65 side chain could readily move to hydrogen-bond with His 157 and act as a proton acceptor in what can be described as a catalytic tetrad. In the active site, Asn 60 is also found to interact with His 157 (Asn 60 N δ 2-His 157 N δ 1, 3.4 Å; Asn 60 N δ 2-His 157 N ϵ 2, 3.7 Å), but it is difficult to imagine it being a suitable proton acceptor because of its nature and position. Therefore, the active site of CMV protease [SEQ ID NO: 1] either consists of a novel triad of Ser 132, His 63 and His 157, or a unique tetrad consisting of Ser 132, His 63, His 157 and Asp 65 that has also never been reported previously (Fig. 41A). In the "catalytic tetrad", His 157 acts as an extra component in this novel "relay" proton transfer mechanism. However, the lack of sequence conservation for Asp 65 (Fig. 1) indicates that this tetrad is not a general model for herpes proteases.

In the active site of the VZV protease [SEQ ID NO: 5] crystal structure, Cys 143 is also found to interact with Ser 120 (Cys 143 S γ -Ser 120 O γ 4.8 Å; Ser 122 O γ -His 139 C ϵ 1, 3.0 Å; Cys 143 S γ -His 52 N ϵ 2 6.0 Å; and Ser 122 O γ -

His 139 Nδ1 2.9 Å), but it is difficult to imagine it being a suitable proton acceptor because of its nature and position. Therefore, the active site of VZV protease consists of a novel triad of Ser 120, His 52 and His 139 of SEQ ID NO: 1 (Fig. 40A).

Overlay of Ser 132 and His 63 of CMV protease (and Ser 120 and His 52 of VZV protease) on Ser 195 and His 57 of the classical serine protease triad in trypsin reveals that His 157 of CMV protease [SEQ ID NO: 1] and His 139 of VZV protease [SEQ ID NO: 5] can be superimposed almost perfectly onto Asp 102 of trypsin (Fig. 41B and Fig. 40B). Not only does this confirm the role of CMV protease His 157 and VZV protease His 139 in catalysis, but it also suggests the possibility of converting this enzyme into one having a normal catalytic triad by replacing His 157 in CMV protease or His 139 in VZV protease with an aspartic acid, which may also require substituting Asp 65 by a non-acidic residue.

In the same overlay, despite a totally different tertiary structure, many interesting conservations can be identified that seem to present a case of convergent evolution. First, Cys 161 for CMV protease and Cys 143 for VZV protease are at an identical position to Cys 42 of trypsin (Fig. 41B and Fig. 40B), making van der Waals interactions with the catalytic residues (Cys 161 S_γ-Ser 132 O_γ, 3.6 Å; Cys 161 S_γ-His 63 N_{ε2}, 4.4 Å in CMV). This surprising conservation, as well as the fact that Cys 161 in CMV protease [SEQ ID NO: 1] and Cys 143 in VZV protease [SEQ ID NO: 5] are absolutely conserved in all herpes proteases, seems to suggest an important role for this amino acid, although mutagenesis studies had shown that it is not essential for the protease activity [Welch I, cited above]. Another similar scenario is found at Ser 134 in CMV protease and Ser 122 in VZV protease, which appear to be at identical positions to Ser 214 of trypsin (Fig. 41B and Fig. 40B).

In the CMV structure of the present invention, Ser 134 interacts strongly with His 157 (Ser 134 O_γ-His 157 N_{ε2}, 2.6 Å; Ser 134 O_γ-His 157 Nδ1, 3.0 Å) by forming a hydrogen bond. In the VZV structure of the invention, Ser 122 interacts strongly with His 139 (Ser 122 O_γ-His 139 N_{ε2}, 2.5 Å) by forming a hydrogen bond. In both CMV and VZV structures, Ser 214 also interacts strongly with Asp 102 in trypsin by forming a hydrogen bond. However, the importance of Ser 134 in CMV protease to the catalytic activity has been undermined by mutagenesis studies [Welch I, cited above], and also the fact that it is an alanine in other herpes virus proteases.

A possible oxyanion hole for the CMV and VZV proteases also exists. In trypsin, the oxyanion is held by the backbone nitrogen atoms of Gly 193 and Ser 195. In the similar region of CMV protease, the construction of the oxyanion hole cannot be fully imitated by the G-X-S-G-G [SEQ ID NO: 14] motif because the backbone arrangements are completely different. However, the main chain nitrogen atom of Arg 165 in CMV protease and Arg 147 in VZV protease is at a nearly identical position as Gly 193 N in trypsin (Figs. 41A and 41B and Figs. 40A and 40B). Also found in the vicinity is a water molecule held by the side chain of Arg 166 and interacting with Leu 20 and Leu 133 (H₂O-Arg 166 NH1, 2.7 Å; H₂O-Arg 166, NZ, 3.2 Å; H₂O-Leu 20 O, 2.6 Å; H₂O-Leu 133 N 3.0 Å). The oxyanion in the structure defined herein may be held only by Arg 165 N, by Arg 165 N and the H₂O molecule. Considering the fact that the two arginines (165 and 166) are absolutely conserved among all herpes proteases (Fig. 1), this general region is suitable for being the oxyanion pocket of CMV [SEQ ID NO: 1] and VZV [SEQ ID NO: 5] proteases.

The active sites of human CMV and VZV proteases sit at a very shallow and mostly exposed region of the protease (Figs. 36B, 41A, 37, 40A). Shallowness of the active site cavity is not really surprising given that the scissile bond (the bond which gets cleaved) recognized by all herpes proteases is between two small amino acid residues (Ala-Ser). Missing around the active site cavity are amino acid residues 143-153 in CMV protease [SEQ ID NO: 1] and aa 139-154 in VZV protease [SEQ ID NO: 5], that are part of a surface loop. This loop contains the so called inactivation or internal (I) site, a cleavage site between Ala 143 and Ala 144 of native human CMV protease as described in Welch I, cited above.

Residue 143 [SEQ ID NO: 1] of the CMV protease of this invention has been mutated to valine to eliminate such processing. Also, it is not clear whether cleavage at the I site is a result of auto-processing or not. Interestingly, a mutant with a five residue deletion around residue 143 was shown to be fully active, but with altered substrate specificity [Welch I, cited above]. Given this loop's proximity to the active site cavity, it may be a flexible flap that is involved in substrate recognition and probably is ordered upon binding of ligands. Similarly, the missing loop containing residues 25-55 may also become ordered upon ligand binding. This is supported by the fact that a mutation of Glu22 in simian CMV protease (corresponding to Glu31 in the human enzyme), has shown altered substrate specificity [Welch I, cited above].

Since the CMV protease structure misses two large loops near the active site, it was difficult to speculate about the substrate binding mode of the enzyme. With the VZV protease structure, the missing loop containing residues 23-45 of SEQ ID NO: 5 becomes ordered, and the structure clearly defines two grooves near the active site that could be important for substrate recognition (Fig. 37). One of the grooves is deeper and wider, and is found in a region that is reminiscent of the S' subsites of classical serine proteases. One side of the groove is delineated by the active site residues, while the other is formed by a side of helix A6, which is also a critical structural feature of the enzyme and will be discussed later. The other groove is relatively narrow. The β-strand B5, including the catalytic triad, is on one side of the shallow depression. The other side is formed by the conserved GRR sequence (Fig. 1) as well as the loop immediately prior to helix AA. This region is also in a position that is not very different from the unprimed (S) subsites in classical serine proteases. Strand B5 being almost parallel to this groove suggests that the substrate peptide (at least P2-P4) could be inserted into the groove with its main chain forming an antiparallel β-sheet with strand B5 and B6. Moreover, several rather exposed hydrophobic residues in the AA loop could also make important interactions with the substrate

protein. Of course, structural studies of enzyme-substrate analog complexes are needed for proving this model.

Given the conservation of amino acid sequence and substrate specificity between CMV, VZV, HSV-1, HSV-2 and other herpes proteases, the structures described herein represent that of the entire family of herpes proteases. These structures are clearly useful in the structure-based design of protease inhibitors, which may be used as therapeutic agents against viral disease. The discovery of the herpes protease catalytic triad, and the catalytic tetrad, permits the design of potent, highly selective protease inhibitors.

F. Mutants and Derivatives

The invention further provides homologues, co-complexes, mutants, derivatives and fragments of the herpes protease crystal structure of the invention.

The term "homologue" means a protein having at least 25% amino acid sequence identity with herpes protease or any functional domain of herpes protease. See Fig. 1.

The term "co-complex" means herpes protease or a mutant or homologue of herpes protease in covalent or non-covalent association with a chemical entity or compound.

The term "mutant" refers to a herpes protease polypeptide, i.e., a polypeptide displaying the biological activity of wild-type protease activity, characterized by the replacement of at least one, or more, amino acids from the wild-type protease sequence. Such a mutant may be prepared, for example, by expression of herpes protease cDNA previously altered in its coding sequence by oligonucleotide-directed mutagenesis.

Herpes protease mutants may also be generated by site-specific incorporation of unnatural amino acids into herpes protease proteins using the general biosynthetic method of C. J. Noren et al, *Science*, 244:182-188 (1989).

In this method, the codon encoding the amino acid of interest in wild-type herpes protease is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis. A suppressor tRNA directed against this codon is then chemically aminoacylated *in vitro* with the desired unnatural amino acid. The aminoacylated tRNA is then added to an *in vitro* translation system to yield a mutant herpes protease enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant herpes protease by expression of herpes protease-encoding cDNAs in auxotrophic *E. coli* strains [W. A. Hendrickson et al, *EMBO J.*, 9(5):1665-1672 (1990)]. In this method, the wild-type or mutagenized herpes protease cDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "heavy atom derivative" refers to derivatives of herpes protease produced by chemically modifying a crystal of herpes protease. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thiomersal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the enzyme [T. L. Blundell and N. L. Johnson, *Protein Crystallography*, Academic Press (1976). See Example I.

The term "fragment", particularly as used in connection with protease fragments, refers to a protease of the invention which contains at least the catalytic active site of the protease, but less than the full length protease. Desirably, the fragment is characterized by a catalytic active site which has the same crystal structure as the active site in the full-length protease. However, a fragment of the invention is not so limited. Such a fragment may contain N-terminal, C-terminal or internal deletions of the protease. Particularly desirable are fragments which are N-terminally truncated proteases. It is currently anticipated that such fragments provide superior resolution or are more easily crystallized.

II. Methods of Identifying Inhibitors of the Novel Protease Crystalline Structure

Another aspect of this invention involves a method for identifying inhibitors of a herpes protease characterized by the crystal structure and novel active site described herein, and the inhibitors themselves. The novel protease crystal structure of the invention permits the identification of inhibitors of protease activity. Such inhibitors may bind to all or a portion of the active site of the herpes protease; or even be competitive non-competitive, or uncompetitive inhibitors; or interfere with dimerization by binding at the interface between the two monomers. Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block protease activity, and thus, herpes viral replication latency, reactivation and/or infection.

One design approach is to probe the herpes protease crystal of the invention with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate herpes protease inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals soaked in or co-crystallized with other molecules allows the determination of where each type of solvent molecule sticks. Molecules that bind tightly to those sites can then be further modified and synthesized and tested for their herpes protease inhibitor activity [J. Travis,

Science, 262:1374 (1993)].

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to or with herpes protease. The time-dependent analysis of structural changes in herpes protease during its interaction with other molecules is permitted. The reaction intermediates of herpes protease can also be deduced from the reaction product in co-complex with herpes protease. Such information is useful to design improved analogues of known herpes protease inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the herpes protease enzyme and herpes protease inhibitor co-complex. This provides a novel route for designing herpes protease inhibitors with both high specificity and stability.

Another approach made possible by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the herpes protease enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy [E. C. Meng et al, J. Comp. Chem., 13:505-524 (1992)].

Because herpes protease may crystallize in more than one crystal form, the structure coordinates of herpes protease, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of herpes protease. They may also be used to solve the structure of herpes protease mutants, herpes protease co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of herpes protease.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of herpes protease, a herpes protease mutant, or a herpes protease co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of herpes protease, may be determined using the herpes protease structure coordinates of this invention as provided in Figs. 1-26. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Thus, the protease structure provided herein permits the screening of known molecules and/or the designing of new molecules which bind to the protease structure, particularly at the active site, via the use of computerized evaluation systems. For example, computer modelling systems are available in which the sequence of the protease, and/or the protease structure (i.e., atomic coordinates of CMV, VZV, HSV-2, or HSV-1 proteases and/or the atomic coordinates of the active site cavity, bond angles, dihedral angles, distances between atoms in the active site region, etc. as provided by Figs. 1-26), may be input. Alternatively, the catalytic site domain crystal structure of a protease of the invention or another fragment of the protease may be input into computer readable form. Thus, for DIP-liganded HSV-2 protease, a machine readable medium may be encoded with data representing the coordinates of Figs. 2, 3, 8, 9, 11, and 12; or Figs. 2, 3, 8, 9, 14, and 15 (Figs. 4 and 5 may be substituted for Figs. 2 and 3 in the process). Similarly, for HSV-1 protease, a machine readable medium may be encoded with data representing the coordinates of Figs. 6, 10 and 13; or Figs. 6, 10 and 16 (as noted Fig. 7 may be substituted for Fig. 6 in this process). For CMV protease, a machine readable medium may be encoded with data representing the coordinates of Figs. 17, 18 and 19; or Figs. 17, 18 and 20 (Fig. 21 may be substituted for Fig. 17 in this process). For VZV protease, a machine readable medium may be encoded with data representing the coordinates of Figs. 22, 24 and 25; or Figs. 22, 24 and 26 (Fig. 23 may be substituted for Fig. 22 in this process). The computer then generates structural details of the site into which a test compound should bind thereby enabling the determination of the complementary structural details of said test compound.

More particularly, the design of compounds that bind to or inhibit herpes protease according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with the herpes protease and, particularly, with the active site thereof. Non-covalent molecular interactions important in the association of herpes protease with its ligands include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with herpes protease. Although certain portions of the compound will not directly participate in this association with herpes protease, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of herpes protease, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with herpes protease.

The potential inhibitory or binding effect of a chemical compound on herpes protease may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and herpes protease, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to herpes protease and inhibit using a suitable assay. In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of herpes protease may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associ-

ate with the individual binding pockets or other areas of herpes protease.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with herpes protease and more particularly with the individual binding pockets of the herpes protease active site or accessory binding site. This process may begin by visual inspection of, for example, the active site on the computer screen based on the herpes protease coordinates in Figs. 2, 3, 6, 8-20, 22, and 24-26. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within a binding pocket of herpes protease. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include the GRID program available from Oxford University, Oxford, UK [P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", *J. Med. Chem.*, 28:849-857 (1985)]; the MCSS program available from Molecular Simulations, Burlington, MA [A. Miranker and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method", *Proteins: Structure, Function and Genetics*, 11:29-34 (1991)]; the AUTODOCK program available from Scripps Research Institute, La Jolla, CA [D. S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", *Proteins: Structure, Function, and Genetics*, 8:195-202 (1990)]; and the DOCK program available from University of California, San Francisco, CA [I. D. Kuntz et al, "A Geometric Approach to Macromolecule-Ligand Interactions", *J. Mol. Biol.*, 161:269-288 (1982)]. Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database, Fine Chemical Database, and CONCORD database [for a review see Rusinko, A., *Chem. Des. Auto. News*, 8:44-47 (1993)].

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of herpes protease. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include the CAVEAT program [P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in *Molecular Recognition in Chemical and Biological Problems*, Special Pub., Royal Chem. Soc: 78, pp. 182-196 (1989)], which is available from the University of California, Berkeley, CA; 3D Database systems such as MACCS-3D database (MDL Information Systems, San Leandro, CA) [see, e.g., Y. C. Martin, "3D Database Searching in Drug Design", *J. Med. Chem.*, 35:2145-2154 (1992)]; and the HOOK program, available from Molecular Simulations, Burlington, MA.

Instead of proceeding to build a herpes protease inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other herpes protease binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known ligand(s). Suitable methods describing such methods include the LUDI program [H.-J. Böhm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", *J. Comp. Aid. Molec. Design*, 6:61-78 (1992)], available from Biosym Technologies, San Diego, CA; the LEGEND program [Y. Nishibata and A. Itai, *Tetrahedron*, 47:8985 (1991)], available from Molecular Simulations, Burlington, MA; and the LeapFrog program, available from Tripos Associates, St. Louis, MO.

Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al, "Molecular Modeling Software and Methods for Medicinal Chemistry", *J. Med. Chem.*, 33:883-894 (1990). See also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", *Current Opinions in Structural Biology*, 2:202-210 (1992). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, e.g., P.S. Farmer, *Drug Design*, Ariens, E.J., ed., Vol. 10, pp 119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; C. Verlinde, *Structure*, 2:577-587 (1994); and I. D. Kuntz, *Science*, 257:1078-1082 (1992). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Thus, using these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds is effectively eliminated.

Once identified by the modelling techniques, the protease inhibitor may be tested for bioactivity using standard techniques. For example, structure of the invention may be used in binding assays using conventional formats to screen inhibitors. Suitable assays for use herein include, but are not limited to, the enzyme-linked immunosorbent assay (ELISA), or a fluorescence quench assay. See, for example, the HSV-1, HSV-2, CMV, and VZV protease activity assays below. Other assay formats may be used; these assay formats are not a limitation on the present invention.

In another aspect, the protease structure of the invention permits the design and identification of synthetic compounds and/or other molecules which have a shape complementary to the conformation of the protease active site of the invention. Using known computer systems, the coordinates of the protease structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed

on the structure of the protease of the invention. Subsequently, suitable candidates identified as above may be screened for the desired protease inhibitory bioactivity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block protease activity, and thus, herpes viral replication.

As used herein the term "natural product molecule" includes all non-synthetic products of nature and includes, but is not limited to, derivatives, extracts or homologs thereof, having, or containing, a bioactive component.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention which is defined by the appended claims.

Example 1: Analysis of the Structure of the HSV-2 Protease

The HSV-2 protease (see Fig. 1, SEQ ID NO: 4) was cloned, expressed and purified as follows:

A. Expression, Purification and Crystallization

HSV-2 protease was expressed in *E. coli* including a 19-residue addition beyond its C-terminal alanine residue [+SEKFKIWGAESAPHHHHHH (SEQ ID NO: 15)]. The hexa-His tag (the six H) allows the high-quality purification of the protein using a Ni²⁺-NTA chromatographic column. The construct also allows the protease to self-process by cleaving the peptide bond between the C-terminal alanine and the first added residue (Ser), thus producing a protein that has the same length as the authentic protease. The protease was further purified using Superdex 75 size exclusion and, if necessary, Q-Sepharose anion exchange chromatography. For the DIP-liganded HSV-2 protease, diisopropyl fluorophosphate inhibitor (DFP) was added to the enzyme and incubated until >98% modification. Excess inhibitor was removed by Sephadex G-25 chromatography.

The DIP-liganded HSV-2 protease was crystallized in 0.1 M NaAcetate buffer pH 5.0 and 10% PEG 4000 (50% w/v). Large crystals are approximately 0.7 mm x 0.3 mm x 0.2 mm in size. The unliganded HSV-2 protease was crystallized in 0.1 M phosphate/Citrate buffer at pH 4.5, 20% PEG 8000. The crystals were 0.3 mm x 0.2 mm x 0.2 mm in size.

B. X-ray Diffraction Characterization

For the liganded and unliganded HSV-2 proteases a crystal was mounted in a sealed glass capillary with a small amount of mother liquor in each end of the capillary. The CuK_α x-ray, having a wavelength of 1.54 Å, was generated by a Siemens-RU200 rotating anode machine operating at 50 KV x 95 mA electric power. The crystal was exposed to the CuK_α x-ray, and the diffracted X-ray was collected by a Siemens multiwire area detector. The DIP-liganded HSV-2 protease crystal diffracted to 2.5 Å resolution. By registering the position and intensity of many tens of thousands of diffraction spots using the computer program XDS, [Kabsch, W., *J. Appl. Cryst.*, 21, pp. 916-924 (1988)] the crystal has been determined to be the orthorhombic space group P2₁2₁2, with a = 71.7 Å, b = 87.4 Å and c = 77.3 Å. By established methods, an asymmetric unit was calculated to have two protein molecules. The crystal contains an estimated 45% solvent. The native data is 91% complete to 2.5 Å with an R_{sym} (Σ||-I|)/Σ(I) of 0.095. The unliganded HSV-2 protease crystal diffracted to 2.8 Å resolution with cell dimensions and space group identical to the DIP-liganded HSV-2 protease crystal. The native data is 94% complete to 2.8 Å with an R_{sym} of 0.095.

C. Heavy Atom Derivative:

Multiple isomorphous replacement (MIR) methods were used as one of the methods in order to obtain phase information of the diffraction data and to solve the three-dimensional atomic structure of the DIP-liganded HSV-2 protease. This involves the identification of derivative crystals containing specifically-bound heavy metal atoms. By testing various heavy metal compounds, the useful derivatives were prepared by soaking the native crystals with 0.1 mM KAuC₄N, 0.4 mM LuCl₃, 0.6 mM PrCl₃, 0.2 mM YbS₄, 0.5 mM GdCl₃, and 0.2 mM SmCl₃ for one to two days. The X-ray diffraction data of the derivative were then collected by the same methods described above. Data collection statistics for native and heavy atom derivatives are shown in Figure 42. Heavy atom positions were identified by difference Patterson and difference Fourier methods using the programs in the XtalView software package [McRee, D.E. *Practical Protein Crystallography*, (San Diego, Academic Press 1993). Heavy atom refinement and determination of an initial set of phases were carried out using the programs in the CCP4 suite [Collaborative Computational Project, Number 4, The CCP4 Suite: Programs for Protein Crystallography *Acta Crystallogr. D* 50, 760-763 (1994)]. The program MLPHARE [Otwinowski, Z. *Isomorphous Replacement and Anomalous Scattering*, 80-86, Daresbury Laboratory, Warrington (1991)] was used for heavy atom phasing. Using the initial phases obtained through the MIR methods, a map of electron density within the crystal unit cell could be calculated. Because electrons are heavily distributed in the immediate vicinity of the centers of atoms, the positions of protein atoms are registered according to the electron density map. The resulting electron density map was interpretable but the phase information from MIR was improved with more phase

information derived from molecular replacement.

D. Molecular Replacement

A molecular replacement solution of the DIP-liganded HSV-2 protease was also identified with the program XPLOR [Brünger, A. T. *X-PLOR Version 3.1: A System for X-ray Crystallography and NMR* (New Haven, Yale University Press; 1992)]. The model for these calculations was a subset of the crystallographic dimer structure of the homologous protease from the VZV alpha-herpes virus (see Example 6 below). Each monomer in the search model was derived from a total of 177 amino acid residues from the VZV protease structure with the sidechains truncated to alanine. The residues of the core secondary structure of the VZV protease were included in the model: residues 11-22, 46-91, 95-124, 137-183 and 189-230 of SEQ ID NO: 5. The rotation function calculation was carried out with data between 15 and 4.0 Å resolution with a maximum search vector length of 38 Å. The top peak in the rotation function from this dimer model was 4.9 s. The translation function was calculated with data between 8 and 4 Å resolution. The top solution was at 9.3 s. Rigid body refinement of the two monomers reduced the R factor to 0.48 for all data to 3.5 Å.

E. Phase Combination

Using difference Fourier methods, phases derived from the molecular replacement solution were consistent with those generated from MIR. The combination of these two sets of phases using the program SIGMAA [Read, R. J. Improved Fourier Coefficients for Maps Using Phases from Partial Structures with Errors *Acta Cryst.* **A42**, 140-149 (1986)] resulted in an overall figure of merit of 0.67. This was followed by one round of non-crystallographic symmetry averaging using the density modification program *dm* [Cowtan, K. Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography **31**, 34-38 (1994)] resulting in an improved overall figure of merit of 0.83. Non-crystallographic symmetry is symmetry that exists locally within the asymmetric unit of the crystal. This information can be used to produce averaged electron density maps in which noise will cancel out and therefore can be used as a phase restriction to improve phasing. The calculated electron density map following this procedure showed side chain density, derived solely from the MIR phases, that was very well-defined and easily interpretable.

F. Model Building and Refinement

The electron density allowed placement of almost all of the side chains in the original model using the program *Xfit* (McRee). Remaining effort was focused on building the missing 27% of the structure that was not part of the molecular replacement model. Two more rounds of density modification with the combined MIR phases allowed placement of an additional alpha helix, several loops and the DIP ligand in the active site. The electron density map resolution was extended to 2.5 Å resolution using *dm*, more residues were added and the model refined using X-PLOR.

When building the model, each of the amino acid residues was manually positioned in its electron density, allowing for a unique position for each atom in the DIP-liganded HSV-2 protease in which each position is defined by a unique set of atomic coordinates (X,Y,Z) as shown in Figure 2A-2F. Starting with these atomic coordinates, a diffraction pattern was calculated and compared to the experimental data. The difference between the calculated and experimentally determined diffraction patterns was monitored by the value of R-factors ($R\text{-factor} = \sum |F_o| - |F_c| / \sum F_o$). The refinement (using XPLOR) of the structural model necessitates adjustments of atomic positions to minimize the R-factor, where a value of about 20% is typical for a good quality protein structure.

Cycles of model building with XTALVIEW and refinement with the computer program XPLOR produce a final model including 217 amino acids with 43 solvent molecules. Three segments of residues are found disordered in the crystal: 104-110, 134-140, and the first 16 residues of the N-terminus [SEQ ID NO: 4]. A total of 14605 reflections were included in the final refinement (10.0 - 2.5 Å), giving an R-factor ($\sum |F_o| - |F_c| / \sum F_o$) of 20.5%. The rms bond length is 0.016 Å and rms bond angle is 1.9°. The program PROCHECK [R. A. Laskowski *et al.*, *J. Appl. Crystallogr.* **26**: 283-291 (1993)] was used to check the stereochemical and geometrical outliers in the final structure, and the result is very satisfactory.

The statistics of structure determination are reported in Fig. 42, where $R_{\text{sym}} = \sum |I - \langle I \rangle| / \sum \langle I \rangle$, I is the observed intensity and $\langle I \rangle$ is the average intensity of multiple observations; $R_{\text{iso}} = \sum |F_{\text{PH}} - F_P| / \sum F_P$, Phasing power = rms isomorphous difference / rms residual lack of closure; $R_{\text{cullis}} = \sum |F_H - F_{H_c}| / \sum |F_H|$, F_H and F_{H_c} are the observed and calculated heavy atom structure factor amplitudes for centric reflections; $R\text{-factor} = \sum |F_o| - |F_c| / \sum F_o$. XPLOR refinement was performed according to A. F. Brünger *et al.*, *Science*, **235**: 458-460 (1987), from 10-2.5 Å. The number of reflections used ($F > 2\sigma$) = 14605, the R-factor was 20.5%; the number of protein atoms (non-H) was 3364; the number of solvent atoms was 43; the RMS bond length was 0.016 Å; and the RMS bond angles = 1.919°. Mean coordinate error (0.3 Å) was performed according to P. V. Luzatti, *Acta Cryst.* **5**: 802-810 (1952). MIR overall mean figure of merit (15-3.0 Å) = 0.62 Å; overall figure of merit after phase combination = 0.67 Å; mean figure of merit following density modification 100-3.0 Å = 0.838 Å.

Using the final atomic coordinates (Figs. 2A-F) one can calculate distances between a pair of atoms, angles

between any three atoms, and dihedral angles between any four atoms, such as listed in Figs. 8A-X, 11A-LLL and 14.

The unliganded HSV-2 protease structure was solved using difference Fourier methods using the refined CIP-liganded HSV-2 protease structure. Since the cell dimensions and space group of the unliganded and liganded (DIP) structure were the same, the DIP-liganded HSV-2 protease structure could be used directly to determine the phases of the unliganded structure, without using heavy atom derivatives or molecular replacement. The unliganded HSV-2 protease model coordinates could then be determined and refined as described for the DIP-liganded HSV-2 protease structure. Three segments of residues were disordered in the unliganded HSV-2 protease structure: 1-16, 104-112, and 134-140 [SEQ ID NO: 4]. A total of 10127 reflections were included in the final refinement (7.0-2.8 Å) giving an R-factor ($\Sigma|F_o| - |F_c| / \Sigma F_o$) of 22.4%. The rms bond length is 0.017 Å and rms bond angle is 2.1°. The program PROCHECK [R. A. Laskowski *et al.*, *J. Appl. Crystallogr.*, 26: 283-291 (1993)] as used to check the stereochemical and geometrical outliers in the final structure, and the result is very satisfactory.

Example 2: Analysis of the Structure of the HSV-1 Protease

The HSV-1 protease (see Fig. 1, SEQ ID NO: 3) was cloned, expressed and purified as follows:

A. Expression, Purification and Crystallization

HSV-1 protease was expressed and purified as described above in Example 1 for HSV-2. HSV-1 was crystallized in 45 mM Tris buffer pH 8.5, 88 mM MgCl₂ and 8.8% PEG 8000 at 4°C.

B. X-ray Diffraction Characterization

A HSV-1 protease crystal was subjected to X-ray diffraction using the techniques described in Example 1 above. The crystal diffracted to 3.5 Å resolution. By registering the position and intensity of many tens of thousands diffraction spots using the computer program XDS [Kabsch, W. *J. Appl. Cryst.* 21, 916-924 (1988)], the crystal has been determined to be the orthorhombic space group P1, with $a = 79.62$ Å $b = 81.18$ Å and $c = 93.36$ Å, $\alpha = 115.49^\circ$ $\beta = 98.36^\circ$ $\gamma = 109.18^\circ$. The native data is 78.4% complete to 3.5 Å with an $R_{\text{sym}} (\Sigma|I(i) - \langle I(i) \rangle| / \Sigma I(i))$ of 0.059. By established methods, an asymmetric unit was calculated to have either six or eight protein molecules (three or four dimers).

C. Molecular Replacement

The HSV-1 protease structure was solved by the method of molecular replacement using the program AMoRe in the CCP4 Suite [Collaborative Computational Project, Number 4 *Acta Crystallogr.* D50, 760-763 (1994)]. The model for these calculations was the entire known crystallographic dimer structure of the highly homologous protease from the HSV-2 alpha-herpes virus complexed with the covalently bound inhibitor DFP. The model was defined as residues: 17-103, 111-133, 141-247 [SEQ ID NO: 3] for each monomer with no inhibitor atoms included. The rotation function calculation was carried out with data between 8 and 4.0 Å resolution with a maximum search vector length of 31.3 Å. Only three pairs of peaks were found with peak height greater than 0.5 (maximum peak height). The pairs of peaks reflected the non-crystallographic symmetry of the dimer. Using data between 8 and 4 Å resolution, the translation function was calculated by fixing the top solution in the P1 cell and searching for a second molecule. This yielded a peak with a correlation coefficient of 41.0% and an R-factor of 38.5%. The top two solutions were then fixed to search for a third, yielding a peak of comparable height to the second solution. A search for a fourth solution showed smaller peaks of all about the same height. To see if there were three or four dimers in the cell a rigid body fit was run to search for four dimers using the top three solutions with several of the similar peaks generated in the last translation function output. The fitting function yielded four peaks with a correlation coefficient of 45.6% and R-factor of 37.1%. Alternatively, when the top three dimer solutions were fit, the correlation coefficient rose to 55.9% with an R-factor of 33.1%. Several other combinations of peaks were tried as controls and none yielded satisfactory results as compared to the top three peaks. A packing diagram was determined and visually inspected using the program Xfit, [McRee, D.E. *Practical Protein Crystallography*, (San Diego, Academic Press, 1993)] showing no overlaps between symmetry related molecules.

D. Model Placement and Refinement

When the molecular replacement solution was placed into the P1 cell, the model was changed slightly in which residues that were different between the two sequences were truncated to alanine to reduce the bias of the HSV-2 protease phases in the calculation of the electron density map. Unfortunately, most of the significant differences between HSV-1 protease and HSV-2 protease in the sequence are present in regions missing in the HSV-2 protease structure [N-terminus and 134-140 of SEQ ID NO: 4], so that many of the changes in the new model, limited by the 3.5 Å resolution, would not be reflected in the electron density map. As a control, to ensure that the map revealed the contributions

of the HSV-1 data, six phenylalanine or tyrosine residues were truncated to alanine on each monomer. Fourier coefficients were calculated using the program SIGMAA [Read, cited above (1986)]. This was followed by phase improvement by non-crystallographic symmetry averaging using the program dm [Cowtan, cited above (1994)]. Non-crystallographic symmetry is symmetry that exists locally within the asymmetric unit of the crystal. This information can be used to produce averaged electron density maps in which noise will cancel out and therefore can be used as a phase restriction to improve phasing.

The calculated electron density map following this procedure showed side chain density that reflected the HSV-1 sequence, within the limits of the resolution, and clearly showed density for the phenylalanine and tyrosine side chains that were omitted from the model, indicating the electron density did reflect the contributions from the HSV-1 protease data.

The residues unique to the HSV-1 protease sequence were built into the model using Xfit (McRee). When building and changing the model, each of the amino acid residues was manually positioned in its electron density, allowing for a unique position for each atom in the HSV-1 protease in which each position is defined by a unique set of atomic coordinates (X, Y, Z) as shown in Figs. 6A-B. Starting with these atomic coordinates, a diffraction pattern was calculated and compared to the experimental data. The difference between the calculated and experimentally determined diffraction patterns was monitored by the value of the R-factor ($R\text{-factor} = \frac{\sum |F_o| - \sum |F_c|}{\sum |F_o|}$). The refinement of the structure was done by rigid body where the fit of the model could be refined by rotation and translation of the entire model. Further positional refinement was not possible because of lack of experimental data as compared to refinement parameters.

The final model has 214 amino acids. Three segments of residues are found disordered in the crystal: 102-110, 134-143, and the first 14 residues of the N-terminus of SEQ ID NO: 3. A total of 12346 reflections were included in the final refinement (10-3.5 Å), giving an R-factor ($\frac{\sum |F_o| - \sum |F_c|}{\sum |F_o|}$) of 36.9%.

Using the final atomic coordinates (Fig. 6) one can calculate distances between a pair of atoms, angles between any three atoms, and dihedral angles between any four atoms, such as listed in Figs. 10A-B, 13A-D and 16.

Example 3: Analysis of the Structure of the CMV Protease

The CMV protease (see Fig. 1, SEQ ID NO: 1) was cloned, expressed and purified as follows:

A. Expression, Purification and Crystallization

CMV A143V protease was expressed and purified as described for HSV-2 and HSV-1. After screening against about a thousand different conditions, the protein was finally crystallized in 30% PEG400 at pH4. Large crystals are approximately 0.4mm x 0.3mm x 0.3mm in size.

B. X-ray Diffraction Characterization

The CMV protease crystal was subjected to x-ray diffraction using the techniques described above for HSV-2 and HSV-1 protease crystals, with the exception that the anode machine was operated at 50 KV x 100 mA electrode power. The crystal diffracted to 3.0 Å resolution. By registering the position and intensity of many tens of thousands diffraction spots using the computer program XGEN, the crystal has been determined to be tetragonal crystal system and P4₃22 space group. The unit cell dimensions are a=b=58.7 Å and c=131.0 Å. By established methods, an asymmetric unit was calculated to have one protein molecule. The crystal contains an estimated 40% solvent.

A higher resolution diffraction data set (2.5 Å) was collected at the Cornell Synchrotron Laboratory (CHESS) A-1 beamline using a CCD detector. The data was processed with the programs DENZO/SCALEPACK [Otwinowski, Z. in *Data Collection and Processing* (eds Sawyer, L., Isaacs, N. Bailey, S.) 56-62, Daresbury Laboratory, Warrington (1993)]. Others were collected with a Siemens multiwire detector on a Siemens CuK_α source and processed with XENGEN [A. J. Howard *et al.*, *J. Appl. Crystallogr.* A47: 110-119 (1994)].

C. Heavy Atom Derivatives:

Using the MIR methods described in Example 1, by testing various heavy metal compounds, the useful derivatives were prepared by soaking the native crystals with saturated MeHgCl (at pH4 or 5), saturated Baker's Dimercury, 1mM UO₂Ac₂, 1mM K₂PtCl₄, 0.5mM LuCl₃ or SmCl₃ for one to four days. The X-ray diffraction data of each of the derivatives were then collected by the same methods described above. Data collection statistics for native and heavy atom derivatives are shown in Fig. 43. Heavy atom positions were identified by difference Patterson and difference Fourier methods using the programs in the CCP4 suite [Collaborative Computational Project, Number 4 *Acta Crystallogr.* D50, 760-763 (1994)]. Anomalous signals from three of the derivatives allowed the determination of the chirality of space group and heavy atom coordinates. Heavy atom refinement and phasing were carried out using the program MLPHARE [Z. Otwinowski, cited above (1991)]. Using the initial phases obtained through the MIR methods, a map of electron density

within the crystal unit cell was calculated. Because electrons are heavily distributed in the immediate vicinity of the centers of atoms, the positions of protein atoms are registered according to the electron density map. The clarity of the electron density map was improved with the methods of solvent flattening, histogram matching and skeletonization.

5 D. Model Building and Refinement

Using the three-dimensional electron density map obtained from above experiments, the polypeptide chain of the CMV protease can be traced without ambiguity. 193 residues (most with side chains) were built using the 3-D computer graphics program XTALVIEW [McRee, D.E., cited above (1993)]. XTALVIEW was used in building models of the CMV protease structure. Each of these 193 amino acids residues was manually positioned in its electron density, allowing for a unique position for each atom in the CMV protease in which each position is defined by a unique set of atomic coordinates (X,Y,Z) as shown in Figs. 17A-E. Starting with these atomic coordinates, a diffraction pattern was calculated and compared to the experimental data. The difference between the calculated and experimentally determined diffraction patterns was monitored by the value of R-factors ($R\text{-factor} = \sum |F_o| - |F_c| / \sum F_o$). The refinement (using XPLORE) of the structural model necessitates adjustments of atomic positions to minimize the R-factor, where a value of below 20% is typical for a good quality protein structure and a value of higher than 20% usually indicates the need of further refinement.

The initial model of CMV protease contains about 70% of the amino acids, having a starting R-factor of 43.8% using the diffraction data from 10 to 3.0 Å. The computer program XPLORE was used to carry out the refinements, and the models were improved gradually after many iteration cycles. The R-factor was decreased to 28.3% after 200 cycles of positional refinement with XPLORE. The final R-factor is 18.7% the CMV protease structure. The program PROCHECK [R. A. Laskowski *et al.*, cited above (1993)] was used to check the stereochemical and geometrical outliers in the final structure, and the result is very satisfactory.

The statistics of structure determination data is reported in Fig. 43, where R_m , R_{iso} , and R_{cutoff} R-factor are as defined in Example 1 above. R_{cutoff} is defined for anomalous amplitudes of non-centric reflections similar to the original R_{cutoff} formula. As described in Example 1, XPLORE refinement was performed according to A. T. Brunger *et al.*, cited above. More particularly, resolution included: 7.0-2.5Å. No. reflections used (>1σ): 7193; R-factor: 0.185; No. protein atoms (non-H): 1604 (202 aa); No. of solvent atoms (non-H): 73; MIR as figure of merit (30-3.2Å): 0.70. Mean coordinates error: 0.4Å; RMS bond length: 0.017Å; RMS bond angle (2.2 degrees). Mean coordinates error was performed according to the SIGMA program [R. Read, *J. Appl. Crystallogr.*, A42: 140-149 (1986)].

Using the final atomic coordinates (Figs. 17A-E) one can calculate distances between a pair of atoms, angles between any three atoms, and dihedral angles between any four atoms, such as listed in Figs. 18A-C, 19A-D and 20.

Example 4: Cloning and Expression of the VZV Protease

The VZV protease gene was located in the complete VZV genome by homology to the protease genes from the HSV-1 and CMV herpes viruses. The VZV genomic sequence used for this analysis was as published by A. Davison & J. Scott, *J. Gen. Virol.*, 67:1759-1816 (1986). The open reading frame for the protease/capsid-encoding gene (equivalent to the HSV-1 UL26 gene) was found to start at base 62,138 and stop at base 60,324 encoding 605 amino acid residues. This open reading frame had been referred to as gene 33 in the above mentioned publication.

The 236 amino acid long protease catalytic domain [SEQ ID NO: 5] was located by identifying the R site that defines the carboxyl-terminal end of all known herpes virus proteases. An alignment of such known R sites is shown in Table I. These cleavage sites are highly conserved (as shown by underlined residues) with cleavage occurring between alanine and serine residues, as indicated by ***.

TABLE I

Protease	R Site Sequence	Sequence ID No:
HSV-1	<u>Tyr-Leu-Gln-Ala</u> *Ser	3
HSV-2	<u>Tyr-Leu-Gln-Ala</u> *Ser	4
CMV	<u>Tyr-Val-Lys-Ala</u> *Ser	1
EBV	<u>Tyr-Leu-Lys-Ala</u> *Ser	6
VZV	<u>Tyr-Leu-Gln-Ala</u> *Ser	5

A. Design of VZV Protease synthetic gene

In an effort to optimize bacterial expression of the VZV protease catalytic domain, a synthetic gene was constructed using codons that are found in proteins highly expressed in *E. coli*. In addition, a number of constructs were made with the goal of facilitating purification of the protein as an active enzyme. Most of the constructs were aimed at producing the authentic species believed to be made during viral infection.

The synthetic gene was designed as follows: A 788 bp VZV protease gene fragment was designed with an NcoI restriction site at the 5' end and XbaI site at the 3' end. These restriction sites are useful for subsequent cloning of the gene fragment in a suitable expression vector. A unique BstE2 restriction site was introduced in the middle of the gene fragment without altering the amino acid sequence. This restriction site was later used to ligate the two synthetic fragments together. It was decided to construct this gene in two portions for the ease of gene synthesis.

The 5' portion of the gene was about 370 bp long and the 3' portion was about 418 bp.

B. Design and synthesis of oligonucleotides

Four megaprimers (primers which are more than 100 bases long) with about 25 bp overlapping ends were designed using the Oligo 4.0 software from National Biosciences Inc. Care was taken to avoid mismatching of overlapping ends. All primers were synthesized on an Applied Biosystem DNA Synthesizer (Model 394) using 40 nM polystyrene columns. Crude oligonucleotide primers were used to assemble the gene fragments. For each portion of the gene, two PCR primers containing unique restriction sites were made using the same DNA synthesizer. These oligonucleotides were referred to as 'nested primers'.

C. Gene Synthesis

The gene synthesis was carried out using the procedure described by Rosen et al, *BioTechniques* 9(3) (1990) with some modifications. For each portion of the gene, two megaprimers oligonucleotides were phosphorylated using the standard kinase procedure [Sambrook et al, *Molecular Cloning. A Laboratory Manual*, 2nd edit., Cold Spring Laboratory, New York (1989)]. In the first polymerase chain reaction (PCR), 0.5 to 1 µg of each of the four megaprimers were mixed together and the PCR was carried out using dNTPs and a mixture of Taq and Vent DNA polymerases (6:1 v/v). Only about 15 cycles of PCR were carried out using the Perkin Elmer PCR 9600 thermocycler (94°C for 30 seconds, 52°C for 30 seconds, 72°C for 45 seconds).

The product of this PCR reaction was used as a template in the second PCR reaction along with 5' and 3' gene specific primers containing unique restriction sites ('nested primers'). PCR reactions was carried out for 25-30 cycles using similar cycle times as above.

About 10 µl of reaction product was analyzed on a 1% agarose gel. PCR products showing a correct size band were then subcloned in the PCR II vector [Invitrogen, San Diego, CA]. The DNA sequence of the synthetic fragments was confirmed by automated DNA sequencing.

D. VZV protease constructs

Six constructs were prepared for the expression of the VZV protease catalytic domain and are illustrated as Figs 45A to 45E [SEQ ID NOS: 7 through 11, respectively]. Authentic VZV protease [SEQ ID NO: 5] contained a protease domain authentic at both amino and carboxyl termini.

H6(N)VZV protease [SEQ ID NO: 7] contained an authentic protease domain preceded at the amino-terminus by six histidine residues (underlined) followed by an enterokinase cleavage site (bold, underlined). The amino-terminal sequence of this construct is: MGHHHHHHSSGH**DDDDK**-MAAE...

LQA-H6(C) VZV protease [SEQ ID NO: 8] contained an authentic protease domain followed by six histidine residues.

LQAS-H6(C) VZV protease [SEQ ID NO: 9] contained an authentic protease domain followed by a serine residue and six histidine residues (underlined).

LQAS-12aa ext H6(C) VZV protease [SEQ ID NO: 10] contains an authentic protease domain followed by a serine residue, 12 residues normally found after the LQAS R-site (bold underlined) and six histidine residues (underlined). The carboxyl-terminal sequence of this construct is: ...LQAS-**TGYGLARITNVN**-HHHHHH.

Delta9 LQAS- 12 aa ext H6(C) VZV protease [SEQ ID NO: 11] contained an authentic protease domain deleted at the amino-terminus (first nine natural residues removed and Cys 10 replaced by Met) and followed at the carboxyl-terminus by a serine residue, 12 residues normally found after the LQAS R-site (bold underlined) and six histidine residues (underlined). The amino-terminus of this construct is MEALYV ...; and the carboxyl-terminal sequence of this construct is: ...LQAS-**TGYGLARITNVN**-HHHHHH.

E. Expression of VZV protease constructs

All constructs were inserted in the *E. coli* expression vector pET16b (Novagen, Madison, WI) in which the inserted gene is under the control of the inducible T7 promoter. The vectors were introduced in the BL21(DE3) *E. coli* strain (Novagen) by standard transformation techniques. The transformed cells were grown to OD₆₅₀=0.5 and then treated with IPTG at 10 mM to induce expression from the T7 promoter. The cells were then aerated for an additional 2 hours and collected by centrifugation. Cell extracts were analyzed for expression by SDS-PAGE followed by Coomassie staining or western blot analysis using a polyclonal antibody against HSV-1 protease, called Anti-95370.

Anti-95370 is a rabbit anti-HSV-1 protease polyclonal antiserum prepared by fusing the complete HSV1 UL26 gene to the C-terminus of a truncated GalK gene in the pOTSFK33 vector described in C. S. Chiang et al, *Clin. Chem.*, 35(6):946-952 (1989). The fusion protein was expressed by conventional protocols and after cell lysis, the insoluble fraction was gel purified using preparative SDS-PAGE. The fusion protein was electroeluted and used to immunize rabbits by standard protocols. The resulting Anti-95370 antisera was shown to cross-react with the VZV protease.

Example 5: Purification of VZV protease constructs

No purification work was done on the authentic VZV protease construct. The other constructs were purified as follows:

A. Purification of H6(N)NZV Protease [SEQ ID NO: 7]

Expression of this protease construct was examined by comparing two hour inductions at 25°C and 37°C. Cells (2-3g) were resuspended in 50 mM Tris pH 8.0, 300 mM NaCl at a ratio of 10 ml/g cells and lysed by sonication on ice. Subsequent purification procedures were performed at 4°C. After centrifugation at 30,000xg, the soluble fraction was further purified by a one hour batch incubation with NiNTA agarose (Qiagen) followed by column chromatography with imidazole washes and elution. Samples were analyzed by Coomassie stained SDS-PAGE and Western blot using Anti-95370 polyclonal antibody described above.

More protease was expressed at 37°C but the majority of the protease was insoluble under both conditions. The soluble protease appeared divided between full length and truncated (identified as C-terminal des30) forms. The majority of the product eluted at 50 mM imidazole rather than the expected 250 mM. The 50 mM eluate was 90% pure, ~90% truncated, active against the JM82 peptide substrate (Ac-HTYLQA*SEKFKMWG; * represents the cleavage site) [SEQ ID NO: 16] and had the correct N-terminal sequence. The activity was attributed to full length product.

B. Purification of LQA-H6(C) VZV Protease [SEQ ID NO: 8] and LQAS-H6(C) VZV Protease [SEQ ID NO: 9]

Cells (5-10g) induced in shake flasks at 25°C and 37°C expressing these constructs were resuspended in 50 mM Tris pH 8.0, 300 mM NaCl at a ratio of 10 ml/g cells and lysed with the Avestin homogenizer (~12,000 psi). The lysate was centrifuged and the soluble fraction was chromatographed on NiNTA agarose. More protease eluted with 50 mM imidazole than with 250 mM imidazole for both constructs induced at 37°C. The majority of product eluted at 250 mM imidazole for LQA-H6(C) VZV protease induced at 25°C. The relative elutions were consistent in RP-HPLC, Coomassie and Western analyses. All products appeared to be of equivalent size.

The products from both constructs had the predicted N-terminal (desMet). The 50 mM eluate from LQAS-H6(C) VZV protease [SEQ ID NO: 9] was concentrated to ~0.6 mg/ml, made 10 mM DTT, 1 mM EDTA and 10% glycerol and incubated at 4°C. Slight activity (<10% specific activity of fully processed protease) against the JM82 peptide substrate was detected 10 days later and confirmed after another 10 days. When the shake flask preparation was repeated and an additional Superdex 75 chromatography step was added, the final product still had only about 10% of the potential activity. Scale-up of LQAS-H6(C) VZV protease [SEQ ID NO: 9] using cells grown in a 10 liter fermentor and induced at OD 0.7 or OD 5.0 at 37°C for 1 hour was unsuccessful.

Coomassie-stained SDS-PAGE gels indicated that lysis was successful but no protease could be detected in NiNTA eluates using RP-HPLC. Western blot detected the best expression with cells induced at OD 0.7 but the majority of the product was insoluble. The same levels of product were detected in the NiNTA agarose load and unbound for the 10L fermented cells suggesting that product did not bind. Product was detected in the load from cells grown in shake flask but not in the unbound fraction suggesting complete capture by NiNTA agarose. The product from all samples had the same apparent molecular weight. The reason for the failure to bind to NiNTA agarose is unknown.

D. Purification of LQAS-12aa ext H6(C) VZV Protease [SEQ ID NO: 10] and delta9 LQAS- 12 aa ext H6(C) VZV Protease [SEQ ID NO: 11]

300g of cells from LQAS-12aa ext H6(C) VZV protease [SEQ ID NO: 10] were resuspended in buffer A (50 mM Tris,

pH8.0, 300 mM NaCl) to a final volume of 3L and the cells were lysed with an Avestin homogenizer at ~12,000 psi. The homogenate was centrifuged for 1 hour, 4°C at 14,000 rpm (30,000 g). The supernatant was collected and added to NiNTA agarose (Qiagen) at a ratio of 1 ml/10g cells. After incubation with rotation at 4°C for 1 hour, the resin was collected by centrifugation for 10 minutes at 3000 rpm. The supernatant was removed with a peristaltic pump and the resin was packed into a Pharmacia 2.6 cm XK column with a 25 ml pipette. The column was washed to baseline absorbance (0.5 mV) with buffer A at 2.5 ml/minute. After washing with 20% B (50 mM imidazole; buffer B is 50 mM Tris, pH8.0, 300 mM NaCl, 250 mM imidazole), the protease was eluted with 100% B (250 mM imidazole). Glycerol was added to the 250 mM eluate to 10%, DTT to 10 mM, and EDTA to 1 mM final concentrations. The sample was filtered with a STE-RIVEX 0.45mm (Millipore) filter and transferred to an Amicon 50 ml stirred cell. After concentration to 5 ml, the sample was diluted to 50 ml with SEC buffer (25 mM HEPES, pH8.0, 50 mM NaCl, 1 mM EDTA, 5 mM DTT) and concentrated to <5 ml. After filtration the sample was stored overnight at 4°C.

The sample was chromatographed on a 2.6 x 60 cm Superdex column equilibrated in SEC buffer. Protease fractions determined by absorbance at 280 nm were pooled and concentrated in a 10 ml stirred cell. Precipitate was removed by centrifugation and the sample was filtered (Millipore ULTRAFREE MC 0.22µm). The VZV protease product was concentrated to 2 mg/ml and diluted with an equal volume of glycerol before storage at -20°C for protease assays. Alternately, protease was concentrated to ~10 mg/ml for crystallography.

The protease product from LQAS-12aa ext H6(C) VZV [SEQ ID NO: 10] was determined to be of the predicted mass by MALDI-MS without the N-terminal Met and with a carboxyl terminus corresponding to authentic protease (i.e., ending with LQA as a result of auto-processing of the 12 amino acid extension at the R site). In fact, it was determined that this construct, which contained a carboxy tail with a hexahistidine tail for binding to NiNTA, following 13 additional amino acids after the LQA mature protein carboxy terminal amino acids, permitted the production of a properly cleaved carboxy terminus for the protein. The protease from delta9 LQAS-12 aa ext H6(C) VZV [SEQ ID NO: 11] had the predicted mass while retaining the N-terminal Met and also ending with LQA. Both proteases were active against the JM82 substrate. Purified protease was a single peak on RP-HPLC and SEC and 95% pure on RP-HPLC.

Protease from delta9 LQAS-12 aa ext H6(C) VZV [SEQ ID NO: 11] was primarily prepared for crystallography (to eliminate structural disorder at the amino terminus) with a typical yield of 4 mg/300 g *E. coli* cells. Protease from LQAS-12aa ext H6(C) VZV [SEQ ID NO: 10] yielded as much as 17 mg/300 g *E. coli* cells.

These modified VZV protein constructs are useful in the crystallization of VZV protease as described below in Example 6, as well as for other biophysical structural studies of VZV protease. The constructs are also useful in biochemical assays to identify compounds which inhibit and/or interact with VZV protease (see Examples 7 and 8 below).

Example 6: Crystallization of the VZV Protease

Protease from delta9 LQAS-12 aa ext H6(C) VZV [SEQ ID NO: 11] was crystallized in 0.1 M phosphate buffer pH6.2 and 2.5 M NaCl. Large crystals are approximately 0.5mm x 0.2mm x 0.2mm in size.

A. X-ray Diffraction Characterization

A VZV protease crystal was subjected to x-ray diffraction characterization, using essentially the same methods as described for CMV. The crystal diffracted to 3.0 Å resolution. By registering the position and intensity of many tens of thousands diffraction spots using the computer program XGEN, the crystal has been determined to be the hexagonal space group P6₃22, with a=b=90.0 Å and c=117.4 Å. By established methods, an asymmetric unit was calculated to have one protein molecule. The crystal contains an estimated 60% solvent. The native data is 90% complete to 3.0 Å with an $R_{\text{merge}} (\sum |I - \langle I \rangle| / \sum I)$ of 0.07.

B. Heavy Atom Derivative

Single isomorphous replacement (SIR) methods were used. The useful derivatives were prepared by soaking the native crystals with 1mM KPt(CN)₂ for one day. Using the initial phases obtained through the SIR methods, a map of electron density within the crystal unit cell could be calculated. Because electrons are heavily distributed in the immediate vicinity of the centers of atoms, the positions of protein atoms are registered according to the electron density map. The clarity of the electron density map could be improved with the methods of solvent flattening, histogram matching and skeletonization. The derivative data is 81% complete to 4.5 Å with an R_{merge} of 0.14 and $R_{\text{iso}} (\sum |F_{\text{PH}} - F_{\text{P}}| / \sum F_{\text{P}})$ of 0.19. This derivative gave a phasing power of 1.2 and $R_{\text{Cullis}} (\sum |F_{\text{H}_0} - F_{\text{H}_c}| / \sum |F_{\text{H}_0}|)$ of 0.79. In this case, the phase information from SIR is not sufficient for structure solution.

C. Molecular Replacement

A molecular replacement (MR) solution using XPLOR [A. Brunger et al. Science 235, 458-460 (1987)] was suc-

cessfully identified only after all the less conserved regions were excluded in the search model which originated from the CMV protease structure. The rotation solution (8.0-4.0 Å) is the highest peak and is 25s above the mean and 1s higher than the second highest peak. Translation searches were carried out in two possible spacegroups P6₂22 and P6₄22, and the latter gave a better solution of 5s in peak height and 52.6% in R-factor (8.0 - 3.0 Å). After rigid body refinement using 8.0-3.0 Å data, the R-factor dropped to 50.6%. When examining the crystal packing, a tight dimer interface was found that corresponds to the same interface in CMV protease. Using the calculated phases from the molecular replacement solution, a heavy atom position was identified using difference Fourier methods that is identical to the one found using difference Patterson methods. This position is in the vicinity of Cys157, which further confirmed the correctness of these results.

D. Phase Combination

The crystal structure of VZV protease was determined using the combination of single isomorphous replacement (SIR) and molecular replacement methods. Neither the SIR map nor the MR map seemed to be interpretable. Combining the phases from both sources, the overall figure of merit was only 0.39 and the map is still quite noisy. Fortunately, there is 60% of solvent in the crystal. After solvent flattening and histogram matching, the electron density map became very clear.

E. Model Building and Refinement

The polypeptide chain of the VZV protease [SEQ ID NO: 5] can be traced without ambiguity using the three-dimensional electron density map obtained from the above experiments and the methods described in Example 3 for CMV above, with the exception that 211 residues (most with side chains) were built.

Cycles of model building with XTALVIEW program and refinement with the XPLOR computer program produce a final model including 211 amino acids without any solvent molecules. Fifteen residues are found disordered in the crystal: 127-136 and 232-236 of SEQ ID NO: 5. A total of 4903 reflections were included in the final refinement (7.0 - 3.0 Å), giving an R-factor ($\sum |F_o| - |F_c| / \sum |F_o|$) of 22.3% without refining temperature factors. The rms bond length is 0.014 Å and rms bond angle is 2.1°. His 52 and His 139 were refined as carrying a single proton at the ND1 atom. The program PROCHECK [R. A. Laskowski et al., *J. Appl. Crystallogr.*, 26: 283-291 (1993)] was used to check the stereochemical and geometrical outliers in the final structure, and the result is very satisfactory.

Using the final atomic coordinates (Figs. 22A-C) one can calculate distances between a pair of atoms, angles between any three atoms, and dihedral angles between any four atoms, such as listed in Figs. 24-26.

EXAMPLE 7: Protease Activity Assays

The biological function of the HSV-2, HSV-1, CMV, and VZV proteases *in vivo* is to specifically cleave the Ala-Ser peptide bonds within a large protein substrate molecule. For routine *in vitro* assay of the protease activity, use of a large protein substrate is inconvenient and very expensive.

A. HSV-2 Protease

For HSV-2 protease, a small peptide substrate having the sequence dabsyl-DNAVEA*SSKAPLK-(dansyl-II)-OH entitled FQ7 (based on VZV m site) [SEQ ID NO: 17] has been synthesized in place of large protein substrate. In the presence of the HSV-2 protease, the FQ7 peptide will be cleaved at the A*S peptide bond, and the product will be the two halves of the substrate. The peptide has been designed so that the cleaved molecules will give rise to strong fluorescence signals.

Therefore, the enzymatic activity of HSV-2 protease can be measured quantitatively by the intensity of the fluorescence signal. This is a very sensitive assay method called fluorescence quenching (FQ). For instance, see, "Principles of Fluorescence Spectroscopy", Lakowicz, J. R., Plenum Press, N.Y. 1983.

In experiments conducted on the HSV-2 protease, the optimized assay conditions call for the use of 520 nM of the HSV-2 protease, 30% of sucrose and 0.8 M citrate. In the presence of added inhibitors, the decreased amount of activity also quantifies the potency of the inhibitors.

B. HSV-1 Protease

For HSV-1 protease, a small peptide substrate having the sequence Ac-HTYLQA*SEKFKMWG entitled JM82 [SEQ ID NO: 16] has been synthesized in place of large protein substrate. In the presence of the HSV-1 protease, the JM82 peptide will be cleaved at the A*S peptide bond, and the product will be the two halves of the substrate. Activity was measured by quantification of the two halves of the substrate using HPLC.

In experiments conducted on the HSV-1 protease, the optimized assay conditions call for the use of 0.3 mg/ml of the HSV-1 protease, 30% of sucrose and 0.8 M citrate in a buffer of 25 mM Hepes (pH 8.0), 50 mM NaCl, 10mM DTT, 1 mM EDTA and 10% Glycerol. In the presence of added inhibitors, the decreased amount of activity also quantifies the potency of the inhibitors.

C. CMV Protease

For CMV protease, a small peptide substrate having the sequence Dbs-RGVVNASSRLAKK-DNS(II) entitled FQ8 [SEQ ID NO: 18] has been synthesized in place of large protein substrate. In the presence of the CMV protease, the FQ8 peptide will be cleaved at the A*S peptide bond, and the product will be the two halves of the substrate. As for HSV-1 and HSV-2 proteases, the peptide substrate has been designed so that the cleaved molecules will give rise to strong fluorescence signals.

In experiments conducted on the CMV protease, the optimised assay conditions call for the use of 20 mM of the CMV protease and 30% of sucrose. In the presence of added inhibitors, the decreased amount of activity also quantifies the potency of the inhibitors.

D. VZV Protease

This assay was performed as described for the proteases above, making use of the FQ7 small peptide substrate. In experiments conducted on the VZV protease, the optimized assay conditions call for the use of 20 nM of the VZV protease, with buffer of 50 mM Hepes, pH8, 150 mM NaCl, 1 mM EDTA, 0.01% PEG with 0.8M citrate/30% sucrose. In the presence of added inhibitors, the decreased amount of activity also quantifies the potency of the inhibitors.

Example 8: Method of Detecting Inhibitors

The three dimensional atomic structure can be readily used as a template for selecting potent inhibitors. Various computer programs and databases are available for the purpose. A good inhibitor should at least have excellent steric and electrostatic complementarity to the target, a fair amount of hydrophobic surface buried and sufficient conformational rigidity to minimize entropy loss upon binding.

There are generally several steps in employing the 3D structure as a template.

First, a target region is defined. In defining a region to target, one can choose the active site cavity of the herpes protease, or any place that is essential to the protease activity. As described above, for HSV-2, HSV-1, CMV and VZV proteases, the crystal structure is determined and therefore spatial and chemical properties of the target region are known.

Second, a small molecule is docked onto the target using one of a variety of methods. Computer databases of three-dimensional structures are available for screening millions of small molecular compounds. A negative image of these compounds is calculated and used to match the shape of the target cavity. The profiles of hydrogen bond donor-acceptor and lipophilic points of these compounds are also used to complement those of the target. One skilled in the art can readily identify many small molecules or fragments as hits.

Third, one may link and extend recognition fragments. Using the hits identified by above procedure, one can incorporate different functional groups or small molecules into a single, larger molecule. The resulting molecule is likely to be more potent and have higher specificity than a single hit. It is also possible to try to improve the "seed" inhibitor by adding more atoms or fragments that will interact with the target protein. The originally defined target region can be readily expanded to allow further necessary extension.

A limited number of promising compounds is selected via this process. The compounds are synthesized and assayed for their inhibitory properties. The success rate is sometimes as high as 20%, and it may still be higher with the rapid progresses in computing methods.

This invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description. Such modifications are intended to fall within the scope of the appended claims.

The disclosures of the patents, patent applications and publications cited herein are incorporated by reference in their entireties.

SEQUENCE LISTING

(1) GENERAL INFORMATION:

- (i) APPLICANT: SmithKline Beecham, Corporation
- (ii) TITLE OF INVENTION: Novel Proteases, Compositions Capable of Binding to Said Site, and Methods of Use Thereof
- (iii) NUMBER OF SEQUENCES: 18
- (iv) CORRESPONDENCE ADDRESS:
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 (C) CITY: King of Prussia
 (D) STATE: Pennsylvania
 (E) COUNTRY: USA
 (F) ZIP: 19406-2799
- (v) COMPUTER READABLE FORM:
 (A) MEDIUM TYPE: Floppy disk
 (B) COMPUTER: IBM PC compatible
 (C) OPERATING SYSTEM: PC-DOS/MS-DOS
 (D) SOFTWARE: PatentIn Release #1.0, Version #1.30
- (vi) CURRENT APPLICATION DATA:
 (A) APPLICATION NUMBER:
 (B) FILING DATE:
 (C) CLASSIFICATION:
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 (B) FILING DATE: 15-MAY-1996
- (vii) PRIOR APPLICATION DATA:
 (A) APPLICATION NUMBER: US 60/022,470
 (B) FILING DATE: 26-JUL-1996
- (vii) PRIOR APPLICATION DATA:
 (A) APPLICATION NUMBER: US 60/024,416
 (B) FILING DATE: 21-AUG-1996
- (vii) PRIOR APPLICATION DATA:
 (A) APPLICATION NUMBER: US 60/030,901
 (B) FILING DATE: 14-NOV-1996
- (vii) PRIOR APPLICATION DATA:
 (A) APPLICATION NUMBER: US 60/035,973
 (B) FILING DATE: 21-JAN-1997
- (vii) PRIOR APPLICATION DATA:
 (A) APPLICATION NUMBER: US 60/039,191
 (B) FILING DATE: 27-FEB-1997
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(2) INFORMATION FOR SEQ ID NO:1:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 256 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

Met Thr Met Asp Glu Gln Gln Ser Gln Ala Val Ala Pro Val Tyr Val
 1 5 10 15
 Gly Gly Phe Leu Ala Arg Tyr Asp Gln Ser Pro Asp Glu Ala Glu Leu
 20 25 30
 Leu Leu Pro Arg Asp Val Val Glu His Trp Leu His Ala Gln Gly Gln
 35 40 45
 Gly Gln Pro Ser Leu Ser Val Ala Leu Pro Leu Asn Ile Asn His Asp
 50 55 60
 Asp Thr Ala Val Val Gly His Val Ala Ala Met Gln Ser Val Arg Asp
 65 70 75 80
 Gly Leu Phe Cys Leu Gly Cys Val Thr Ser Pro Arg Phe Leu Glu Ile
 85 90 95
 Val Arg Arg Ala Ser Glu Lys Ser Glu Leu Val Ser Arg Gly Pro Val
 100 105 110
 Ser Pro Leu Gln Pro Asp Lys Val Val Glu Phe Leu Ser Gly Ser Tyr
 115 120 125
 Ala Gly Leu Ser Leu Ser Ser Arg Arg Cys Asp Asp Val Glu Ala Ala
 130 135 140
 Thr Ser Leu Ser Gly Ser Glu Thr Thr Pro Phe Lys His Val Ala Leu
 145 150 155 160
 Cys Ser Val Gly Arg Arg Arg Gly Thr Leu Ala Val Tyr Gly Arg Asp
 165 170 175
 Pro Glu Trp Val Thr Gln Arg Phe Pro Asp Leu Thr Ala Ala Asp Arg
 180 185 190
 Asp Gly Leu Arg Ala Gln Trp Gln Arg Cys Gly Ser Thr Ala Val Asp
 195 200 205
 Ala Ser Gly Asp Pro Phe Arg Ser Asp Ser Tyr Gly Leu Leu Gly Asn
 210 215 220
 Ser Val Asp Ala Leu Tyr Ile Arg Glu Arg Leu Pro Lys Leu Arg Tyr
 225 230 235 240
 Asp Lys Gln Leu Val Gly Val Thr Glu Arg Glu Ser Tyr Val Lys Ala
 245 250 255

(2) INFORMATION FOR SEQ ID NO:2:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 230 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2:

Met Ser Lys Val Trp Val Gly Gly Phe Leu Cys Val Tyr Gly Glu Glu
 1 5 10 15
 Pro Ser Glu Glu Cys Leu Ala Leu Pro Arg Asp Thr Val Gln Lys Glu
 20 25 30
 Leu Gly Ser Gly Asn Ile Pro Leu Pro Leu Asn Ile Asn His Asn Glu
 35 40 45
 Lys Ala Thr Ile Gly Met Val Arg Gly Leu Phe Asp Leu Glu His Gly
 50 55 60
 Leu Phe Cys Val Ala Gln Ile Gln Ser Gln Thr Phe Met Asp Ile Ile
 65 70 75 80
 Arg Asn Ile Ala Gly Lys Ser Lys Leu Ile Thr Ala Gly Ser Val Ile
 85 90 95
 Glu Pro Leu Pro Pro Asp Pro Glu Ile Glu Cys Leu Ser Ser Ser Phe
 100 105 110
 Pro Gly Leu Ser Leu Ser Ser Lys Val Leu Gln Asp Glu Asn Leu Asp
 115 120 125
 Gly Lys Pro Phe Phe His His Val Ser Val Cys Gly Val Gly Arg Arg
 130 135 140
 Pro Gly Thr Ile Ala Ile Phe Gly Arg Glu Ile Ser Trp Ile Leu Asp
 145 150 155 160
 Arg Phe Ser Cys Ile Ser Glu Ser Glu Lys Arg Gln Val Leu Glu Gly
 165 170 175
 Val Asn Val Tyr Ser Gln Gly Phe Asp Glu Asn Leu Phe Ser Ala Asp
 180 185 190
 Leu Tyr Asp Leu Leu Ala Asp Ser Leu Asp Thr Ser Tyr Ile Arg Lys
 195 200 205
 Arg Phe Pro Lys Leu Gln Leu Asp Lys Gln Leu Cys Gly Leu Ser Lys
 210 215 220
 Cys Thr Tyr Ile Lys Ala
 225 230

(2) INFORMATION FOR SEQ ID NO:3:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 247 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:3:

5 Met Ala Ala Asp Ala Pro Gly Asp Arg Met Glu Glu Pro Leu Pro Asp
 1 5 10 15
 Arg Ala Val Pro Ile Tyr Val Ala Gly Phe Leu Ala Leu Tyr Asp Ser
 20 25 30
 10 Gly Asp Ser Gly Glu Leu Ala Leu Asp Pro Asp Thr Val Arg Ala Ala
 35 40 45
 Leu Pro Pro Asp Asn Pro Leu Pro Ile Asn Val Asn His Arg Ala Gly
 50 55 60
 15 Cys Glu Val Gly Arg Val Leu Ala Val Val Asp Asp Pro Arg Gly Pro
 65 70 75 80
 Phe Phe Val Gly Leu Ile Ala Cys Val Gln Leu Glu Arg Val Leu Glu
 85 90 95
 20 Thr Ala Ala Ser Ala Ala Ile Phe Glu Arg Arg Gly Pro Pro Leu Ser
 100 105 110
 Arg Glu Glu Arg Leu Leu Tyr Leu Ile Thr Asn Tyr Leu Pro Ser Val
 115 120 125
 25 Ser Leu Ala Thr Lys Arg Leu Gly Gly Glu Ala His Pro Asp Arg Thr
 130 135 140
 Leu Phe Ala His Val Ala Leu Cys Ala Ile Gly Arg Arg Leu Gly Thr
 145 150 155 160
 30 Ile Val Thr Tyr Asp Thr Gly Leu Asp Ala Ala Ile Ala Pro Phe Arg
 165 170 175
 His Leu Ser Pro Ala Ser Arg Glu Gly Ala Arg Arg Leu Ala Ala Glu
 180 185 190
 35 Ala Glu Leu Ala Leu Ser Gly Arg Thr Trp Ala Pro Gly Val Glu Ala
 195 200 205
 Leu Thr His Thr Leu Leu Ser Thr Ala Val Asn Asn Met Met Leu Arg
 210 215 220
 40 Asp Arg Trp Ser Leu Val Ala Glu Arg Arg Arg Gln Ala Gly Ile Ala
 225 230 235 240
 Gly His Thr Tyr Leu Gln Ala
 245

(2) INFORMATION FOR SEQ ID NO:4:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 247 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:4:

Met Ala Ser Ala Glu Met Arg Glu Arg Leu Glu Ala Pro Leu Pro Asp
 1 5 10 15
 Arg Ala Val Pro Ile Tyr Val Ala Gly Phe Leu Ala Leu Tyr Asp Ser
 20 25 30
 Gly Asp Pro Gly Glu Leu Ala Leu Asp Pro Asp Thr Val Arg Ala Ala
 35 40 45
 Leu Pro Pro Glu Asn Pro Leu Pro Ile Asn Val Asn His Arg Ala Arg
 50 55 60
 Cys Glu Val Gly Arg Val Leu Ala Val Val Asn Asp Pro Arg Gly Pro
 65 70 75 80
 Phe Phe Val Gly Leu Ile Ala Cys Val Gln Leu Glu Arg Val Leu Glu
 85 90 95
 Thr Ala Ala Ser Ala Ala Ile Phe Glu Arg Arg Gly Pro Ala Leu Ser
 100 105 110
 Arg Glu Glu Arg Leu Leu Tyr Leu Ile Thr Asn Tyr Leu Pro Ser Val
 115 120 125
 Ser Leu Ser Thr Lys Arg Arg Gly Asp Glu Val Pro Pro Asp Arg Thr
 130 135 140
 Leu Phe Ala His Val Ala Leu Cys Ala Ile Gly Arg Arg Leu Gly Thr
 145 150 155 160
 Ile Val Thr Tyr Asp Thr Ser Leu Asp Ala Ala Ile Ala Pro Phe Arg
 165 170 175
 His Leu Asp Pro Ala Thr Arg Glu Gly Val Arg Arg Glu Ala Ala Glu
 180 185 190
 Ala Glu Leu Ala Leu Ala Gly Arg Thr Trp Ala Pro Gly Val Glu Ala
 195 200 205
 Leu Thr His Thr Leu Leu Ser Thr Ala Val Asn Asn Met Met Leu Arg
 210 215 220
 Asp Arg Trp Ser Leu Val Ala Glu Arg Arg Arg Gln Ala Gly Ile Ala
 225 230 235 240
 Gly His Thr Tyr Leu Gln Ala
 245

(2) INFORMATION FOR SEQ ID NO:5:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 236 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS:
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:5:

EP 0 807 687 A2

5 Met Ala Ala Glu Ala Asp Glu Glu Asn Cys Glu Ala Leu Tyr Val Ala
 1 5 10 15
 Gly Leu Tyr Ala Leu Tyr Ser Lys Asp Glu Gly Glu Leu Asn Ile Thr
 20 25 30
 Pro Glu Ile Val Arg Ser Ala Leu Pro Pro Thr Ser Lys Ile Pro Ile
 35 40 45
 Asn Ile Asp His Arg Lys Asp Cys Val Val Gly Glu Val Ile Ala Ile
 50 55 60
 Ile Glu Asp Ile Arg Gly Pro Phe Phe Leu Gly Ile Val Arg Cys Pro
 65 70 75 80
 Gln Leu His Ala Val Leu Phe Glu Ala Ala His Ser Asn Phe Phe Gly
 85 90 95
 Asn Arg Asp Ser Val Leu Ser Pro Leu Glu Arg Ala Leu Tyr Leu Val
 100 105 110
 Thr Asn Tyr Leu Pro Ser Val Ser Leu Ser Ser Lys Arg Leu Ser Pro
 115 120 125
 Asn Glu Ile Pro Asp Gly Asn Phe Phe Thr His Val Ala Leu Cys Val
 130 135 140
 Val Gly Arg Arg Val Gly Thr Val Val Asn Tyr Asp Cys Thr Pro Glu
 145 150 155 160
 Ser Ser Ile Glu Pro Phe Arg Val Leu Ser Met Glu Ser Lys Ala Arg
 165 170 175
 Leu Leu Ser Leu Val Lys Asp Tyr Ala Gly Leu Asn Lys Val Trp Lys
 180 185 190
 Val Ser Glu Asp Lys Leu Ala Lys Val Leu Leu Ser Thr Ala Val Asn
 195 200 205
 Asn Met Leu Leu Arg Asp Arg Trp Asp Val Val Ala Lys Arg Arg Arg
 210 215 220
 Glu Ala Gly Ile Met Gly His Val Tyr Leu Gln Ala
 225 230 235

(2) INFORMATION FOR SEQ ID NO:6:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 235 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS:
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:6:

50 Met Val Gln Ala Pro Ser Val Tyr Val Cys Gly Phe Val Glu Arg Pro
 1 5 10 15
 Asp Ala Pro Pro Lys Asp Ala Cys Leu His Leu Asp Pro Leu Thr Val
 20 25 30

Lys Ser Gln Leu Pro Leu Lys Lys Pro Leu Pro Leu Thr Val Glu His
 35 40 45
 5 Leu Pro Asp Ala Pro Val Gly Ser Val Phe Gly Leu Tyr Gln Ser Arg
 50 55 60
 Ala Gly Leu Phe Ser Ala Ala Ser Ile Thr Ser Gly Asp Phe Leu Ser
 65 70 75 80
 10 Leu Leu Asp Ser Ile Tyr His Asp Cys Asp Ile Ala Gln Ser Gln Arg
 85 90 95
 Leu Pro Leu Pro Arg Glu Pro Lys Val Glu Ala Leu His Ala Trp Leu
 100 105 110
 15 Pro Ser Leu Ser Leu Ala Ser Leu His Pro Asp Ile Pro Gln Thr Thr
 115 120 125
 Ala Asp Gly Gly Lys Leu Ser Phe Phe Asp His Val Ser Ile Cys Ala
 130 135 140
 20 Leu Gly Arg Arg Arg Gly Thr Thr Ala Val Tyr Gly Thr Asp Leu Ala
 145 150 155 160
 Trp Val Leu Lys His Phe Ser Asp Leu Glu Pro Ser Ile Ala Ala Gln
 165 170 175
 25 Ile Glu Asn Asp Ala Asn Ala Ala Lys Arg Glu Ser Gly Cys Pro Glu
 180 185 190
 Asp His Pro Leu Pro Leu Thr Lys Leu Ile Ala Lys Ala Ile Asp Ala
 195 200 205
 Gly Phe Leu Arg Asn Arg Val Glu Thr Leu Arg Gln Asp Arg Gly Val
 210 215 220
 30 Ala Asn Ile Pro Ala Glu Ser Tyr Leu Lys Ala
 225 230 235

(2) INFORMATION FOR SEQ ID NO:7:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 254 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:7:

Met Gly His His His His His Ser Ser Gly His Ile Asp Asp Asp
 1 5 10 15
 Asp Lys Met Ala Ala Glu Ala Asp Glu Glu Asn Cys Glu Ala Leu Tyr
 20 25 30
 Val Ala Gly Leu Tyr Ala Leu Tyr Ser Lys Asp Glu Gly Glu Leu Asn
 35 40 45
 50 Ile Thr Pro Glu Ile Val Arg Ser Ala Leu Pro Pro Thr Ser Lys Ile
 50 55 60

EP 0 807 687 A2

Pro Ile Asn Ile Asp His Arg Lys Asp Cys Val Val Gly Glu Val Ile
65 70 75 80

Ala Ile Ile Glu Asp Ile Arg Gly Pro Phe Phe Leu Gly Ile Val Arg
85 90 95

Cys Pro Gln Leu His Ala Val Leu Phe Glu Ala Ala His Ser Asn Phe
100 105 110

Phe Gly Asn Arg Asp Ser Val Leu Ser Pro Leu Glu Arg Ala Leu Tyr
115 120 125

Leu Val Thr Asn Tyr Leu Pro Ser Val Ser Leu Ser Ser Lys Arg Leu
130 135 140

Ser Pro Asn Glu Ile Pro Asp Gly Asn Phe Phe Thr His Val Ala Leu
145 150 155 160

Cys Val Val Gly Arg Arg Val Gly Thr Val Val Asn Tyr Asp Cys Thr
165 170 175

Pro Glu Ser Ser Ile Glu Pro Phe Arg Val Leu Ser Met Glu Ser Lys
180 185 190

Ala Arg Leu Leu Ser Leu Val Lys Asp Tyr Ala Gly Leu Asn Lys Val
195 200 205

Trp Lys Val Ser Glu Asp Lys Leu Ala Lys Val Leu Leu Ser Thr Ala
210 215 220

Val Asn Asn Met Leu Leu Arg Asp Arg Trp Asp Val Val Ala Lys Arg
225 230 235 240

Arg Arg Glu Ala Gly Ile Met Gly His Val Tyr Leu Gln Ala
245 250

(2) INFORMATION FOR SEQ ID NO:8:

- (i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 242 amino acids
 - (B) TYPE: amino acid
 - (C) STRANDEDNESS:
 - (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:8:

Met Ala Ala Glu Ala Asp Glu Glu Asn Cys Glu Ala Leu Tyr Val Ala
1 5 10 15

Gly Leu Tyr Ala Leu Tyr Ser Lys Asp Glu Gly Glu Leu Asn Ile Thr
20 25 30

Pro Glu Ile Val Arg Ser Ala Leu Pro Pro Thr Ser Lys Ile Pro Ile
35 40 45

Asn Ile Asp His Arg Lys Asp Cys Val Val Gly Glu Val Ile Ala Ile
50 55 60

Ile Glu Asp Ile Arg Gly Pro Phe Phe Leu Gly Ile Val Arg Cys Pro
65 70 75 80

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5 Gln Leu His Ala Val Leu Phe Glu Ala Ala His Ser Asn Phe Phe Gly
 85 90 95
 Asn Arg Asp Ser Val Leu Ser Pro Leu Glu Arg Ala Leu Tyr Leu Val
 100 105 110
 Thr Asn Tyr Leu Pro Ser Val Ser Leu Ser Ser Lys Arg Leu Ser Pro
 115 120 125
 10 Asn Glu Ile Pro Asp Gly Asn Phe Phe Thr His Val Ala Leu Cys Val
 130 135 140
 Val Gly Arg Arg Val Gly Thr Val Val Asn Tyr Asp Cys Thr Pro Glu
 145 150 155 160
 Ser Ser Ile Glu Pro Phe Arg Val Leu Ser Met Glu Ser Lys Ala Arg
 15 165 170 175
 Leu Leu Ser Leu Val Lys Asp Tyr Ala Gly Leu Asn Lys Val Trp Lys
 180 185 190
 Val Ser Glu Asp Lys Leu Ala Lys Val Leu Leu Ser Thr Ala Val Asn
 195 200 205
 20 Asn Met Leu Leu Arg Asp Arg Trp Asp Val Val Ala Lys Arg Arg Arg
 210 215 220
 Glu Ala Gly Ile Met Gly His Val Tyr Leu Gln Ala His His His His
 225 230 235 240
 25 His His

(2) INFORMATION FOR SEQ ID NO:9:

30 (i) SEQUENCE CHARACTERISTICS:
 (A) LENGTH: 243 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

35 (ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:9:

40 Met Ala Ala Glu Ala Asp Glu Glu Asn Cys Glu Ala Leu Tyr Val Ala
 1 5 10 15
 Gly Leu Tyr Ala Leu Tyr Ser Lys Asp Glu Gly Glu Leu Asn Ile Thr
 20 25 30
 45 Pro Glu Ile Val Arg Ser Ala Leu Pro Pro Thr Ser Lys Ile Pro Ile
 35 40 45
 Asn Ile Asp His Arg Lys Asp Cys Val Val Gly Glu Val Ile Ala Ile
 50 55 60
 50 Ile Glu Asp Ile Arg Gly Pro Phe Phe Leu Gly Ile Val Arg Cys Pro
 65 70 75 80
 Gln Leu His Ala Val Leu Phe Glu Ala Ala His Ser Asn Phe Phe Gly
 85 90 95

55

EP 0 807 687 A2

Asn Arg Asp Ser Val Leu Ser Pro Leu Glu Arg Ala Leu Tyr Leu Val
100 105 110
5 Thr Asn Tyr Leu Pro Ser Val Ser Leu Ser Ser Lys Arg Leu Ser Pro
115 120 125
Asn Glu Ile Pro Asp Gly Asn Phe Phe Thr His Val Ala Leu Cys Val
130 135 140
10 Val Gly Arg Arg Val Gly Thr Val Val Asn Tyr Asp Cys Thr Pro Glu
145 150 155 160
Ser Ser Ile Glu Pro Phe Arg Val Leu Ser Met Glu Ser Lys Ala Arg
165 170 175
15 Leu Leu Ser Leu Val Lys Asp Tyr Ala Gly Leu Asn Lys Val Trp Lys
180 185 190
Val Ser Glu Asp Lys Leu Ala Lys Val Leu Leu Ser Thr Ala Val Asn
195 200 205
Asn Met Leu Leu Arg Asp Arg Trp Asp Val Val Ala Lys Arg Arg Arg
210 215 220
20 Glu Ala Gly Ile Met Gly His Val Tyr Leu Gln Ala Ser His His His
225 230 235 240
His His His

(2) INFORMATION FOR SEQ ID NO:10:

- (i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 255 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS:
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:10:

Met Ala Ala Glu Ala Asp Glu Glu Asn Cys Glu Ala Leu Tyr Val Ala
1 5 10 15
40 Gly Leu Tyr Ala Leu Tyr Ser Lys Asp Glu Gly Glu Leu Asn Ile Thr
20 25 30
Pro Glu Ile Val Arg Ser Ala Leu Pro Pro Thr Ser Lys Ile Pro Ile
35 40 45
45 Asn Ile Asp His Arg Lys Asp Cys Val Val Gly Glu Val Ile Ala Ile
50 55 60
Ile Glu Asp Ile Arg Gly Pro Phe Phe Leu Gly Ile Val Arg Cys Pro
65 70 75 80
50 Gln Leu His Ala Val Leu Phe Glu Ala Ala His Ser Asn Phe Phe Gly
85 90 95
Asn Arg Asp Ser Val Leu Ser Pro Leu Glu Arg Ala Leu Tyr Leu Val
100 105 110

Thr Asn Tyr Leu Pro Ser Val Ser Leu Ser Ser Lys Arg Leu Ser Pro
 115 120 125
 Asn Glu Ile Pro Asp Gly Asn Phe Phe Thr His Val Ala Leu Cys Val
 130 135 140
 Val Gly Arg Arg Val Gly Thr Val Val Asn Tyr Asp Cys Thr Pro Glu
 145 150 155 160
 Ser Ser Ile Glu Pro Phe Arg Val Leu Ser Met Glu Ser Lys Ala Arg
 165 170 175
 Leu Leu Ser Leu Val Lys Asp Tyr Ala Gly Leu Asn Lys Val Trp Lys
 180 185 190
 Val Ser Glu Asp Lys Leu Ala Lys Val Leu Leu Ser Thr Ala Val Asn
 195 200 205
 Asn Met Leu Leu Arg Asp Arg Trp Asp Val Val Ala Lys Arg Arg Arg
 210 215 220
 Glu Ala Gly Ile Met Gly His Val Tyr Leu Gln Ala Ser Thr Gly Tyr
 225 230 235 240
 Gly Leu Ala Arg Ile Thr Asn Val Asn His His His His His
 245 250 255

(2) INFORMATION FOR SEQ ID NO:11:

(i) SEQUENCE CHARACTERISTICS:
 (A) LENGTH: 246 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:11:

Met Glu Ala Leu Tyr Val Ala Gly Leu Tyr Ala Leu Tyr Ser Lys Asp
 1 5 10 15
 Glu Gly Glu Leu Asn Ile Thr Pro Glu Ile Val Arg Ser Ala Leu Pro
 20 25 30
 Pro Thr Ser Lys Ile Pro Ile Asn Ile Asp His Arg Lys Asp Cys Val
 35 40 45
 Val Gly Glu Val Ile Ala Ile Ile Glu Asp Ile Arg Gly Pro Phe Phe
 50 55 60
 Leu Gly Ile Val Arg Cys Pro Gln Leu His Ala Val Leu Phe Glu Ala
 65 70 75 80
 Ala His Ser Asn Phe Phe Gly Asn Arg Asp Ser Val Leu Ser Pro Leu
 85 90 95
 Glu Arg Ala Leu Tyr Leu Val Thr Asn Tyr Leu Pro Ser Val Ser Leu
 100 105 110
 Ser Ser Lys Arg Leu Ser Pro Asn Glu Ile Pro Asp Gly Asn Phe Phe
 115 120 125

Thr His Val Ala Leu Cys Val Val Gly Arg Arg Val Gly Thr Val Val
 130 135 140
 Asn Tyr Asp Cys Thr Pro Glu Ser Ser Ile Glu Pro Phe Arg Val Leu
 145 150 155 160
 Ser Met Glu Ser Lys Ala Arg Leu Leu Ser Leu Val Lys Asp Tyr Ala
 165 170 175
 Gly Leu Asn Lys Val Trp Lys Val Ser Glu Asp Lys Leu Ala Lys Val
 180 185 190
 Leu Leu Ser Thr Ala Val Asn Asn Met Leu Leu Arg Asp Arg Trp Asp
 195 200 205
 Val Val Ala Lys Arg Arg Arg Glu Ala Gly Ile Met Gly His Val Tyr
 210 215 220
 Leu Gln Ala Ser Thr Gly Tyr Gly Leu Ala Arg Ile Thr Asn Val Asn
 225 230 235 240
 His His His His His His
 245

(2) INFORMATION FOR SEQ ID NO:12:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 5 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS:
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: peptide

(ix) FEATURE:

- (A) NAME/KEY: Modified-site
- (B) LOCATION: 3
- (D) OTHER INFORMATION: /note= "Amino acid in position 3 can be Cys or Ser"

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:12:

Gly Xaa Xaa Gly Gly
1 5

(2) INFORMATION FOR SEQ ID NO:13:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 4 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS:
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: peptide

(ix) FEATURE:

- (A) NAME/KEY: Modified-site
- (B) LOCATION: 4
- (D) OTHER INFORMATION: /note= "Amino acid in position 4 can be Met or Ala"

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:13:

Gly Thr Ser Xaa
1

(2) INFORMATION FOR SEQ ID NO:14:

- (i) SEQUENCE CHARACTERISTICS:
 (A) LENGTH: 5 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: peptide

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:14:

Gly Xaa Ser Gly Gly
1 5

(2) INFORMATION FOR SEQ ID NO:15:

- (i) SEQUENCE CHARACTERISTICS:
 (A) LENGTH: 19 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS: single
 (D) TOPOLOGY: unknown

(ii) MOLECULE TYPE: peptide

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:15:

Ser Glu Lys Phe Lys Ile Trp Gly Ala Glu Ser Ala Pro His His His
1 5 10 15
His His His

(2) INFORMATION FOR SEQ ID NO:16:

- (i) SEQUENCE CHARACTERISTICS:
 (A) LENGTH: 14 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: peptide

(ix) FEATURE:

- (A) NAME/KEY: Modified-site
 (B) LOCATION: 1
 (D) OTHER INFORMATION: /note= "His in amino acid position
 1 is modified to contain an acetyl group"

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:16:

His Thr Tyr Leu Gln Ala Ser Glu Lys Phe Lys Met Trp Gly
1 5 10

(2) INFORMATION FOR SEQ ID NO:17:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 13 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: peptide

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:17:

Asp Asn Ala Val Glu Ala Ser Ser Lys Ala Pro Leu Lys
 1 5 10

(2) INFORMATION FOR SEQ ID NO:18:

(i) SEQUENCE CHARACTERISTICS:

- (A) LENGTH: 13 amino acids
 (B) TYPE: amino acid
 (C) STRANDEDNESS:
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: peptide

(ix) FEATURE:

- (A) NAME/KEY: Modified-site
 (B) LOCATION: 1

(D) OTHER INFORMATION: /note= "Arg at amino acid position 1 is modified to contain a dabsyl group"

(ix) FEATURE:

- (A) NAME/KEY: Modified-site
 (B) LOCATION: 13

(D) OTHER INFORMATION: /note= "Lys at amino acid position 13 is modified to contain a dansyl-II g..."

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:18:

Arg Gly Val Val Asn Ala Ser Ser Arg Leu Ala Lys Lys
 1 5 10

Claims

1. A composition comprising a herpes virus protease in crystalline form.
2. The composition according to claim 1 wherein said protease has an active site cavity formed by at least the amino acids Ser, His and His.
3. The composition according to claim 1 wherein said protease is a dimer.
4. A heavy atom derivative of a herpes virus protease crystal.
5. The composition according to claim 1 wherein said protease is selected from the group consisting of herpes simplex virus (HSV)-2 and HSV-1 and has an active site formed by the amino acids Ser 129, His 61, and His 148 cor-

responding to SEQ ID NO: 3 and 4.

6. The composition according to claim 1 wherein said protease is HSV-2 and said active site is characterized by the coordinates selected from the group consisting of the coordinates of Figures 2 and 3, the coordinates of Figures 8 and 9, and the coordinates of Figures 11 and 12.
7. The composition according to claim 5 wherein the protease is HSV-1, and said active site further includes amino acids Ala 131, Cys 152, Arg 156 and Arg 157 corresponding to SEQ ID NO: 3.
8. The composition according to claim 5 wherein said protease is HSV-1 and said active site is characterized by the coordinates selected from the group consisting of the coordinates of Figures 6 or 7, the coordinates of Figure 10, and the coordinates of Figure 13.
9. The composition according to claim 1 wherein said protease is human cytomegalovirus protease (CMV) and has an active site cavity formed by at least the amino acids Ser 132, His 64, and His 157 corresponding to SEQ ID NO: 1.
10. The composition according to claim 9, wherein said CMV protease active site is formed by the amino acids Ser 132, His 63, His 157, and Asp 65 corresponding to SEQ ID NO: 1.
11. The composition according to claim 9, wherein said CMV protease active site is characterized by the coordinates selected from the group consisting of the coordinates of Figure 17 or Figure 21, the coordinates of Figure 18, and the coordinates of Figure 19.
12. The composition according to claim 1, wherein said protease is varicella zoster virus (VZV) and has an active site cavity formed by at least the amino acids Ser 120, His 52, His 139, and Lys 54 corresponding to SEQ ID NO: 5.
13. The composition according to claim 12, wherein said VZV protease active site is formed by the amino acids Ser 120, His 52, His 139, Lys 54, Ser 122, Cys 143, Arg 147, and Arg 148 corresponding to SEQ ID NO: 5.
14. The composition according to claim 11, wherein said VZV protease active site is characterized by the coordinates selected from the group consisting of the coordinates of Figure 22 or Figure 23, the coordinates of Figure 24, and the coordinates of Figure 25.
15. An isolated, properly folded herpes simplex virus (HSV) 2 protease molecule, or fragment thereof, having a conformation comprising a catalytically active site formed by the interaction of three amino acids Serine, Histidine and Histidine, said active site defined by the protein coordinates of Figures 2 and 3, the distances between atoms of Figures 8 and 9, and the bond angles between interresidue atoms of Figures 11 and 12.
16. The HSV-2 protease molecule according to claim 15, wherein said molecule is a monomer characterized by a 7-stranded β -barrel core with seven α helices, as illustrated in Figures 29A,B,C, and 31.
17. The HSV-2 protease molecule according to claim 15, wherein said molecule is a dimer characterized by the dimer interface of Fig.27 A,B, and C.
18. An isolated, properly folded herpes simplex virus (HSV) 1 protease molecule, or fragment thereof, having a conformation comprising a catalytically active site formed by the interaction of three amino acids Serine, Histidine and Histidine, said active site defined by the protein coordinates of Figure 6, the distances between atoms of Figure 10, and the bond angles between interresidue atoms of Figure 13.
19. The HSV-1 protease molecule according to claim 18, wherein said molecule is a monomer characterized by a 7-stranded β -barrel core with seven α helices, as illustrated in Figures 30 A,B, and 31.
20. The HSV-1 protease molecule according to claim 18 wherein said molecule is a dimer characterized by the dimer interface of Fig.28 A, and B.
21. An isolated, properly folded cytomegalovirus (CMV) protease molecule, or fragment thereof, having a conformation comprising a catalytically active site formed by the interaction of three amino acids Serine, Histidine and Histidine, said active site defined by the protein coordinates of Figure 17, the distances between atoms of Figure 18, and the

bond angles between interresidue atoms of Figure 19.

22. The CMV protease molecule according to claim 21, wherein said molecule is a monomer characterized by a 7-stranded β -barrel core with seven α helices, as illustrated in Figures 32 A, 32B, and 34.

23. The CMV protease molecule according to claim 21, wherein said molecule is a dimer characterized by the dimer interface of Fig. 36.

24. An isolated, properly folded varicella zoster virus (VZV) protease molecule, or fragment thereof, having a conformation comprising a catalytically active site formed by the interaction of three amino acids Serine, Histidine and Histidine; said active site defined by the protein coordinates of Figure 22; the distances between atoms of Figure 24, and the bond angles between interresidue atoms of Figure 25.

25. The VZV protease molecule according to claim 24 wherein said molecule is a monomer characterized by a 7-stranded β -barrel core with eight α helices, as illustrated in Figures 33A, 33B, and 35.

26. The VZV protease molecule according to claim 24 wherein said molecule is a dimer characterized by the dimer interface of Fig. 37.

27. A peptide, peptidomimetic, synthetic or natural product molecule which binds with the active site cavity of a herpes virus protease composition, derivative or molecule of any of claims 1 to 26.

28. A method of identifying an inhibitor compound capable of binding to, and inhibiting the proteolytic activity of, a herpes protease, or any other protease characterized by the Ser-His-His catalytic triad, said method comprising:

introducing into a suitable computer program information defining an active site conformation of a herpes protease molecule comprising a catalytically active site formed by at least the interaction of three amino acids Serine, Histidine and Histidine, wherein said program displays the three-dimensional structure thereof; creating a three dimensional representation of the active site cavity in said computer program; displaying and superimposing the model of said test compound on the model of said active site; assessing whether said test compound model fits spatially into the active site; incorporating said test compound in a biological protease activity assay for a protease characterized by said active site; and determining whether said test compound inhibits proteolytic activity in said assay.

29. The method according to claim 28, wherein the protease is liganded or unliganded herpes simplex virus (HSV)2 according to any of claims 15 to 17.

30. The method according to claim 28, wherein the protease is herpes simplex virus (HSV) 1 according to any of claims 18 to 20.

31. The method according to claim 28, wherein the protease is cytomegalovirus according to any of claims 21 to 23.

32. The method according to claim 28, wherein the protease is varicella zoster virus according to any of claims 24 to 27.

33. A peptide, peptidomimetic, synthetic or natural product molecule identified by the method of claim 28.

34. A method for solving a crystal form comprising using the structural coordinates of herpes protease crystal or portions thereof, to solve a crystal form of a mutant, homologue or co-complex of said protease by molecular rearrangement.

35. A method of drug design comprising using the structural coordinates of a herpes protease crystal to computationally evaluate a chemical entity for associating with the active site of a herpes virus protease.

36. The method according to claim 35, wherein said entity is a competitive, non-competitive or uncompetitive inhibitor, binds to or inhibits the proteolytic activity of a herpes virus protease.

37. The method of drug design comprising using the structure coordinates of a herpes virus protease to identify an

intermediate in a chemical reaction between said protease and a compound which is a substrate or inhibitor of said protease.

38. The method according to claims 25 or 37, wherein said structure coordinates are selected from the group consisting the coordinates of Figures 2, 3, 6; 8-20, 22 and 22-26.

39. A method for identifying inhibitors which competitively bind to the dimeric interface of a herpes virus protease molecule or fragment thereof, which protease is characterized by a catalytically active site formed by the interaction of three amino acids Serine, Histidine and Histidine, said method comprising the steps of:

providing the coordinates of said active site, and dimeric interface of said protease to a computerized modeling system;

identifying compounds which will bind to, or interfere with, the dimeric interface; and

screening the compounds identified for protease inhibitory bioactivity.

40. A method for identifying inhibitors which competitively bind to the active site of a herpes virus protease molecule or fragment thereof characterized by a catalytically active site formed by the interaction of three amino acids Serine, Histidine and Histidine, said method comprising the steps of:

providing the coordinates of said active site of the protease to a computerized modeling system;

identifying compounds which will bind to the structure; and

screening the compounds identified for protease inhibitory bioactivity.

41. The method according to claim 40, wherein the protease is liganded or unliganded herpes simplex virus (HSV) 2 according to any of claims 15 to 17.

42. The method according to claim 40, wherein the protease is herpes simplex virus (HSV) 1 according to any of Claims 18 to 20.

43. The method according to claim 40, wherein the protease is cytomegalovirus (CMV) according to any of claims 21 to 23.

44. The method according to claim 40, wherein the protease is varicella zoster virus (VZV) according to any of claims 24 to 26.

45. A modified varicella zoster virus (VZV) protease selected from the group consisting of the sequence of Fig. 45A SEQ ID NO: 7, the sequence of Fig. 45B SEQ ID NO: 8, the sequence of Fig. 45C SEQ ID NO: 9, the sequence of Fig. 45D SEQ ID NO: 10, and the sequence of Fig. 45E SEQ ID NO: 11.

46. A method of forming a crystal of VSV protease comprising crystallizing a modified VSV protease of claim 45.

47. The method according to claim 46, wherein said VSV protease has the sequence of Fig. 45E SEQ ID NO: 11.

48. In a bioassay for identifying inhibitors of VSV protease, wherein said bioassay comprises the step of exposing a VZV protease to a candidate inhibitor, the improvement comprising using as said VSV protease a protease of claim 45.

49. A method for purifying a varicella zoster virus (VZV) protease with an intact mature carboxy terminal sequence of LQA, said method comprising purifying an authentic VZV sequence with an amino acid sequence interposed between said LQA terminal amino acids and a hexahistidine sequence on an NiNTA column.

50. The method according to claim 49, wherein said VZV sequence is that of Fig. 45E SEQ ID NO: 11.

51. A method for purifying a cytomegalovirus (CMV) protease with an intact mature carboxy terminal sequence of LQA, said method comprising purifying an authentic CMV sequence with an amino acid sequence interposed between said LQA terminal amino acids and a hexahistidine sequence on an NiNTA column.

52. A method for purifying a herpes simplex virus (HSV) 1 protease with an intact mature carboxy terminal sequence of LQA, said method comprising purifying an authentic HSV1 sequence with an amino acid sequence interposed

between said LQA terminal amino acids and a hexahistidine sequence on an NiNTA column.

53. A method for purifying a herpes simplex virus (HSV) 2 protease with an intact mature carboxy terminal sequence of LQA, said method comprising purifying an authentic HSV2 sequence with an amino acid sequence interposed
5 between said LQA terminal amino acids and a hexahistidine sequence on an NiNTA column.

54. A computer readable medium having stored thereon a model of the crystal structure of the catalytic site domain of a herpes protease.

10 55. A protease crystal structure characterized by a catalytic site triad comprising Serine, Histidine and Histidine.

56. The protease crystal structure according to claim 55, wherein said structure is a truncated herpes protease.

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Fig. 1

Herpes Proteases Sequence Alignment Based on Structures

	B1		A1		B2	
CMV	MTMDEQQSQA	VAPVYVGGFL	ARYDQSPDEA	ELLPLRDVVE	HWLHAQQGQG	PSLSVALPLN 60
HHV6		MSKWVVGGL	CVYGEESPSE	CLALPRDTVQ	KEL---GSGN	----IPLPEN
EBV		MVQ	APSVYVCGFV	ERPDAPPKDA	CLHLDPLTVK	SQPLK---KPLPLT
HSV1	MAADAPG	DRMEEPLPDR	AVPIYVAGFL	ALYDSGDSGE	-LALDPDTVR	AALPPD---NPLPIN
HSV2	MASAEMR	ERLEAPLPDR	AVPIYVAGFL	ALYDSGDPGE	-LALDPDTVR	AALPPE---NPLPIN
VZV		MAAEADEEN	CEALYVAGYL	ALY-SKDEGE	-LINITPEIVR	SALPPT---SKIPIN
	B3		A2		A3	
CMV	INHDDTAVVG	HVAAMQSVRD	GLFCLGCVTS	PRFLEIVRRA	SEKS--ELVSRG	PVSPQLPDKV VEFLSGSYAG 130
HHV6	INHNEKATEG	MVRGLFDLEH	GLFCVAQIQS	QTFMDIIRNI	AGKS-KLITAGS	VIEPLPPDPE IECLSSSFPG
EBV	VEHLPDAPVG	SVFGLYQSRA	GLFSAASITS	GDFLSLDSI	YHDC--DIAQSQ	RL-PLPREPK VEALHAWLPS
HSV1	VNHRAGCEVG	RVLAVVDDPR	GPFFVGLIAC	VQLERVLETA	ASAAIFERRGP	PLSRE--ERL LYLTITNYLPS
HSV2	VNHRARCEVG	RVLAVVNDPR	GPFFVGLIAC	VQLERVLETA	ASAAIFERRGP	ALSRE--ERL LYLTITNYLPS
VZV	IDHRKDCVVG	EVIAIIEDIR	GPFFLGIVRC	PQLHAVLFEA	AHSNFFGNRDSV	-LSPL--ERA LYLVTNYLPS
	B5		B6		A4	
CMV	LSLSSRRRCDD	VEAATSLSGS	ETTPFKHVAL	CSVGRRRGTL	AVYGRDPEWV	TQRFDDLTA DRDGLRAQWQ 200
HHV6	LSLSSK----	VLQDENLDGK	--PFFHHVSV	CGVGRRRPGTI	AIFGREISWI	LDRFSCISES EKQVLEGVN
EBV	LSLASLHPD-	-IPQTTADGG	KLSEFFDHVSI	CALGRRRGTT	AVYGTDLAWV	LKHFSDLPS IAAQIENDAN
HSV1	VSLATKRLGG	EAHPDR----	--TLFAHVAL	CAIGRRRLGTI	VTYDTGLDAA	IAPFRHLSPA SREGARRLAA
HSV2	VSLSTKRRGD	EVPPDR----	--TLFAHVAL	CAIGRRRLGTI	VTYDTSLDAA	IAPFRHLSPA TREGVRREAA
VZV	VSLSSKRLSP	NEIPDG----	--NFTTHVAL	CVVGRRVGTI	VNYDCTPES	IEPFRVLSME SKARLLSLVK
	A6		A7		A5	
CMV	RCGSTAVDAS	GDP-FRSDSYG	LLGNSVDALY	IRERLPKLRYD	KQLVGVTER	ESYVKA 256
HHV6	VYSQGFDENL	FS---ADLYD	LLADSLDTSY	IRKRFPKLQLD	KQLCGLS-K	CTVIKA
EBV	AAKRESGCPE	DHP---LPLTK	LIAKAIDAGF	LRNRVETLRQD	RGVANIPA-	ESYLKA
HSV1	EAEALSGRT	WAPGVEALHT	LLSTAVNNMM	LRDRWSLVAER	RRQAGIAGH	-TYLQA
HSV2	EAEALAGRT	WAPGVEALHT	LLSTAVNNMM	LRDRWSLVAER	RRQAGIAGH	-TYLQA
VZV	DYAGLN--KV	WKVSEDKLAKV	LLSTAVNNML	LRDRWDVVAKR	RREAGIMGH	-VYLQA

Fig. 2A

Atom	AA	No.	X	Y	Z	OCC	B-Factor
72	N	LEU A 27	35.736	25.246	1.206	1.00	5.10
73	CA	LEU A 27	35.022	24.000	1.421	1.00	6.35
74	CB	LEU A 27	34.241	23.628	0.173	1.00	4.80
75	CG	LEU A 27	32.753	23.867	0.051	1.00	2.00
76	CD1	LEU A 27	32.147	24.549	1.270	1.00	2.00
77	CD2	LEU A 27	32.558	24.628	-1.224	1.00	2.00
78	C	LEU A 27	36.089	22.929	1.732	1.00	8.64
79	O	LEU A 27	35.816	21.898	2.340	1.00	8.93
151	N	LEU A 38	38.679	12.044	3.012	1.00	26.85
152	CA	LEU A 38	38.221	13.442	2.935	1.00	20.79
153	CB	LEU A 38	38.298	14.040	4.341	1.00	19.20
154	CG	LEU A 38	37.385	13.373	5.387	1.00	19.62
155	CD1	LEU A 38	37.541	14.052	6.749	1.00	14.44
156	CD2	LEU A 38	35.921	13.404	4.918	1.00	12.06
157	C	LEU A 38	38.902	14.349	1.898	1.00	18.61
158	O	LEU A 38	38.318	15.277	1.372	1.00	19.33
314	N	ASP A 60	24.054	21.586	10.505	1.00	20.34
315	CA	ASP A 60	24.514	20.256	10.991	1.00	32.81
316	CB	ASP A 60	24.285	20.194	12.514	1.00	40.06
317	CG	ASP A 60	25.230	19.225	13.226	1.00	46.11
318	OD1	ASP A 60	26.474	19.401	13.129	1.00	48.62
319	OD2	ASP A 60	24.718	18.292	13.900	1.00	50.43
320	C	ASP A 60	23.866	19.032	10.254	1.00	36.61
321	O	ASP A 60	23.201	18.163	10.839	1.00	39.35
322	N	HIS A 61	24.053	19.024	8.937	1.00	41.05
323	CA	HIS A 61	23.564	17.952	8.013	1.00	47.22
324	CB	HIS A 61	24.547	16.770	7.982	1.00	47.84
325	CG	HIS A 61	25.792	17.052	7.195	1.00	49.75
326	CD2	HIS A 61	25.965	17.423	5.907	1.00	51.27

Fig. 2B

Atom	AA	No.	X	Y	Z	OCC	B-Factor
327	ND1	HIS A 61	27.049	17.028	7.757	1.00	51.98
328	CE1	HIS A 61	27.943	17.377	6.847	1.00	53.59
329	NE2	HIS A 61	27.311	17.623	5.713	1.00	50.47
330	C	HIS A 61	22.126	17.445	8.142	1.00	49.08
331	O	HIS A 61	21.680	16.560	7.392	1.00	53.07
782	N	SER A 127	32.204	26.649	11.275	1.00	2.00
783	CA	SER A 127	32.669	25.783	10.146	1.00	2.00
784	CB	SER A 127	33.270	24.508	10.731	1.00	2.00
785	OG	SER A 127	34.258	24.800	11.690	1.00	2.49
786	C	SER A 127	31.674	25.377	9.036	1.00	2.00
787	O	SER A 127	30.463	25.486	9.164	1.00	2.00
788	N	VAL A 128	32.222	24.903	7.920	1.00	2.00
789	CA	VAL A 128	31.380	24.368	6.809	1.00	4.25
790	CB	VAL A 128	31.641	24.922	5.406	1.00	5.15
791	CG1	VAL A 128	30.631	25.964	5.077	1.00	14.62
792	CG2	VAL A 128	33.039	25.411	5.261	1.00	3.69
793	C	VAL A 128	31.775	22.937	6.678	1.00	5.33
794	O	VAL A 128	32.845	22.503	7.066	1.00	8.22
795	P1	SEI A 129	31.695	17.762	7.461	1.00	8.79
796	O3	SEI A 129	31.372	17.687	9.055	1.00	11.54
797	O4	SEI A 129	31.616	16.285	6.832	1.00	7.78
798	O5	SEI A 129	30.630	18.671	6.720	1.00	9.57
799	C5	SEI A 129	30.226	17.113	9.752	1.00	10.71
800	C6	SEI A 129	30.679	16.036	10.741	1.00	11.64
801	C7	SEI A 129	29.405	18.197	10.462	1.00	2.00
802	C8	SEI A 129	31.769	15.900	5.468	1.00	5.88
803	C9	SEI A 129	30.614	14.989	5.035	1.00	10.05
804	C10	SEI A 129	33.106	15.201	5.285	1.00	10.92
805	N	SEI A 129	30.916	22.193	6.024	1.00	7.00

Fig. 2C

Atom	AA	No.	X	Y	Z	OCC	B-Factor
ATOM 806	CA	SEI A 129	31.186	20.804	5.818	1.00	4.93
ATOM 807	C	SEI A 129	30.516	20.458	4.534	1.00	3.57
ATOM 808	O	SEI A 129	29.305	20.529	4.410	1.00	5.86
ATOM 809	CB	SEI A 129	30.536	20.063	6.956	1.00	4.94
ATOM 810	O2	SEI A 129	33.031	18.359	7.260	1.00	17.04
ATOM 811	N	LEU A 130	31.332	20.138	3.541	1.00	4.70
ATOM 812	CA	LEU A 130	30.814	19.774	2.219	1.00	6.09
ATOM 813	CB	LEU A 130	31.825	20.095	1.127	1.00	8.94
ATOM 814	CG	LEU A 130	31.491	19.566	-0.273	1.00	2.00
ATOM 815	CD1	LEU A 130	30.306	20.309	-0.854	1.00	2.00
ATOM 816	CD2	LEU A 130	32.720	19.745	-1.157	1.00	4.46
ATOM 817	C	LEU A 130	30.500	18.314	2.158	1.00	6.28
ATOM 818	O	LEU A 130	31.293	17.487	2.554	1.00	12.07
ATOM 819	N	SER A 131	29.320	17.984	1.669	1.00	8.28
ATOM 820	CA	SER A 131	28.978	16.564	1.504	1.00	8.85
ATOM 821	CB	SER A 131	27.618	16.283	2.096	1.00	5.12
ATOM 822	OG	SER A 131	27.656	16.625	3.465	1.00	19.47
ATOM 823	C	SER A 131	29.022	16.243	-0.003	1.00	10.39
ATOM 824	O	SER A 131	28.527	16.996	-0.846	1.00	11.22
ATOM 825	N	THR A 132	29.664	15.127	-0.333	1.00	12.55
ATOM 826	CA	THR A 132	29.790	14.670	-1.728	1.00	16.62
ATOM 827	CB	THR A 132	31.271	14.437	-2.085	1.00	15.84
ATOM 828	OG1	THR A 132	31.893	13.713	-1.019	1.00	16.85
ATOM 829	CG2	THR A 132	32.004	15.768	-2.282	1.00	14.99
ATOM 830	C	THR A 132	29.028	13.347	-1.849	1.00	19.10
ATOM 831	O	THR A 132	28.990	12.558	-0.903	1.00	18.44
ATOM 893	N	HIS A 148	25.733	19.031	-0.862	1.00	12.59
ATOM 894	CA	HIS A 148	25.300	20.234	-0.089	1.00	10.63
ATOM 895	CB	HIS A 148	23.987	19.958	0.619	1.00	10.37

Fig. 2D

<u>Atom</u>	<u>AA</u>	<u>No.</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>OCC B-Factor</u>
ATOM	CG	HIS A 148	24.047	18.808	1.577	1.00 19.25
ATOM	CD2	HIS A 148	23.866	17.477	1.389	1.00 23.23
ATOM	ND1	HIS A 148	24.283	18.967	2.926	1.00 26.01
ATOM	CE1	HIS A 148	24.244	17.791	3.527	1.00 23.57
ATOM	NE2	HIS A 148	23.992	16.869	2.615	1.00 25.40
ATOM	C	HIS A 148	26.358	20.634	0.949	1.00 12.85
ATOM	O	HIS A 148	27.342	19.912	1.222	1.00 10.96
ATOM	N	VAL A 149	26.145	21.803	1.547	1.00 9.18
ATOM	CA	VAL A 149	27.067	22.274	2.595	1.00 7.72
ATOM	CB	VAL A 149	27.780	23.596	2.229	1.00 9.50
ATOM	CG1	VAL A 149	28.036	23.637	0.751	1.00 11.54
ATOM	CG2	VAL A 149	27.012	24.800	2.695	1.00 11.06
ATOM	C	VAL A 149	26.277	22.435	3.880	1.00 7.39
ATOM	O	VAL A 149	25.120	22.861	3.904	1.00 6.80
ATOM	N	ALA A 150	26.916	22.032	4.964	1.00 7.47
ATOM	CA	ALA A 150	26.302	22.093	6.270	1.00 5.81
ATOM	CB	ALA A 150	26.244	20.710	6.876	1.00 2.00
ATOM	C	ALA A 150	27.130	23.017	7.142	1.00 5.80
ATOM	O	ALA A 150	28.347	23.019	7.091	1.00 15.09
ATOM	N	LEU A 151	26.443	23.901	7.853	1.00 5.33
ATOM	CA	LEU A 151	27.083	24.817	8.800	1.00 3.39
ATOM	CB	LEU A 151	26.157	25.991	9.072	1.00 5.70
ATOM	CG	LEU A 151	26.241	27.301	8.296	1.00 7.34
ATOM	CD1	LEU A 151	26.854	27.107	6.939	1.00 3.41
ATOM	CD2	LEU A 151	24.841	27.925	8.241	1.00 4.66
ATOM	C	LEU A 151	27.204	23.934	10.043	1.00 3.49
ATOM	O	LEU A 151	26.316	23.128	10.340	1.00 2.65
ATOM	N	CYS A 152	28.306	24.058	10.770	1.00 5.06
ATOM	CA	CYS A 152	28.482	23.240	11.983	1.00 2.81

Fig. 2E

<u>Atom</u>	<u>AA</u>	<u>No.</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>OCC</u>	<u>B-Factor</u>
925 ATOM	CB	CYS A 152	28.884	21.838	11.561	1.00	2.00
926 ATOM	SG	CYS A 152	30.351	21.833	10.545	1.00	12.33
927 ATOM	C	CYS A 152	29.525	23.887	12.880	1.00	3.00
928 ATOM	O	CYS A 152	30.084	24.917	12.574	1.00	6.88
934 ATOM	N	ILE A 154	32.449	22.278	14.209	1.00	3.33
935 ATOM	CA	ILE A 154	33.791	21.856	13.831	1.00	6.57
936 ATOM	CB	ILE A 154	34.519	21.214	15.065	1.00	13.23
937 ATOM	CG2	ILE A 154	35.849	20.661	14.679	1.00	15.20
938 ATOM	CG1	ILE A 154	34.742	22.247	16.184	1.00	17.08
939 ATOM	CD1	ILE A 154	35.736	23.354	15.845	1.00	21.42
940 ATOM	C	ILE A 154	33.620	20.837	12.671	1.00	8.07
941 ATOM	O	ILE A 154	32.935	19.820	12.802	1.00	6.60
942 ATOM	N	GLY A 155	34.206	21.179	11.516	1.00	7.25
943 ATOM	CA	GLY A 155	34.138	20.338	10.335	1.00	8.29
944 ATOM	C	GLY A 155	35.202	19.269	10.364	1.00	9.30
945 ATOM	O	GLY A 155	36.071	19.289	11.239	1.00	11.83
946 ATOM	N	ARG A 156	35.176	18.363	9.393	1.00	8.85
947 ATOM	CA	ARG A 156	36.182	17.277	9.359	1.00	10.92
948 ATOM	CB	ARG A 156	35.496	15.967	8.996	1.00	17.70
949 ATOM	CG	ARG A 156	34.400	15.595	9.973	1.00	20.67
950 ATOM	CD	ARG A 156	34.337	14.120	10.205	1.00	29.56
951 ATOM	NE	ARG A 156	34.168	13.376	8.965	1.00	41.87
952 ATOM	CZ	ARG A 156	34.645	12.149	8.765	1.00	50.41
953 ATOM	NH1	ARG A 156	34.438	11.536	7.603	1.00	51.55
954 ATOM	NH2	ARG A 156	35.340	11.537	9.724	1.00	54.89
955 ATOM	C	ARG A 156	37.420	17.537	8.476	1.00	10.96
956 ATOM	O	ARG A 156	38.466	16.913	8.597	1.00	13.19
957 ATOM	N	ARG A 157	37.278	18.458	7.547	1.00	9.18
958 ATOM	CA	ARG A 157	38.395	18.809	6.689	1.00	7.21

Fig. 2F

Atom	AA	No.	X	Y	Z	OCC	B-Factor
ATOM	959	CB ARG A 157	37.889	19.001	5.268	1.00	3.14
ATOM	960	CG ARG A 157	37.587	17.685	4.570	1.00	5.26
ATOM	961	CD ARG A 157	37.501	17.781	3.034	1.00	5.80
ATOM	962	NE ARG A 157	36.109	17.989	2.665	1.00	9.28
ATOM	963	CZ ARG A 157	35.294	17.125	2.068	1.00	10.11
ATOM	964	NH1 ARG A 157	35.612	15.920	1.630	1.00	7.28
ATOM	965	NH2 ARG A 157	34.036	17.269	2.355	1.00	17.52
ATOM	966	C ARG A 157	39.054	20.074	7.280	1.00	9.04
ATOM	967	O ARG A 157	38.454	20.808	8.066	1.00	7.54
ATOM	3320	OH2 HOH WAT1	34.674	20.373	6.663	1.00	2.00
ATOM	3355	OH2 HOH WAT2	34.176	20.162	3.994	1.00	17.52

Fig. 3A

Residue Atom	X	Y	Z	B
27 LEU N	35.91	25.23	1.03	8.63
27 LEU CA	35.20	23.98	1.32	9.80
27 LEU CB	34.35	23.49	0.15	7.49
27 LEU CG	32.94	24.00	-0.06	7.63
27 LEU CD1	32.31	24.50	1.21	2.13
27 LEU CD2	32.97	25.06	-1.07	9.69
27 LEU C	36.25	22.93	1.61	9.77
27 LEU O	35.93	21.86	2.11	12.13
38 LEU N	38.77	12.21	3.00	25.79
38 LEU CA	38.44	13.62	2.95	22.29
38 LEU CB	38.81	14.28	4.28	21.83
38 LEU CG	37.90	13.88	5.44	22.40
38 LEU CD1	36.48	13.63	4.92	18.69
38 LEU CD2	38.44	12.61	6.10	24.95
38 LEU C	39.06	14.39	1.80	21.48
38 LEU O	38.38	15.13	1.08	19.95
60 ASP N	24.14	21.54	10.22	6.21
60 ASP CA	24.72	20.29	10.69	9.27
60 ASP CB	24.50	20.16	12.22	12.92
60 ASP CG	25.64	19.40	12.93	18.52
60 ASP OD1	26.78	19.39	12.40	23.62
60 ASP OD2	25.43	18.84	14.04	15.83
60 ASP C	24.21	19.05	9.96	10.71
60 ASP O	23.88	18.06	10.57	12.47
61 HIS N	24.13	19.11	8.64	12.79
61 HIS CA	23.68	17.98	7.81	14.32
61 HIS C	22.24	17.54	7.92	17.79
61 HIS O	21.85	16.59	7.25	20.60
61 HIS CB	24.59	16.76	7.96	10.25
61 HIS CG	26.00	17.01	7.52	12.30
61 HIS ND1	26.39	17.08	6.21	13.19

Fig. 3B

Residue Atom	X	Y	Z	B
61 HIS CD2	27.10	17.30	8.26	11.24
61 HIS NE2	28.16	17.57	7.41	13.47
61 HIS CE1	27.69	17.42	6.18	11.79
127 SER N	32.35	26.51	11.23	7.34
127 SER CA	32.78	25.64	10.14	7.69
127 SER CB	33.33	24.36	10.71	7.69
127 SER OG	34.45	24.61	11.53	12.66
127 SER C	31.75	25.27	9.10	7.85
127 SER O	30.58	25.48	9.30	11.85
128 VAL N	32.23	24.80	7.95	4.94
128 VAL CA	31.36	24.32	6.89	5.12
128 VAL CB	31.40	25.12	5.59	2.60
128 VAL CG1	31.07	26.50	5.86	11.40
128 VAL CG2	32.70	25.03	4.93	2.00
128 VAL C	31.84	22.93	6.62	7.19
128 VAL O	32.97	22.58	6.92	11.48
129 SER N	30.97	22.13	6.04	6.97
129 SER CA	31.32	20.78	5.73	7.38
129 SER CB	30.73	19.90	6.80	8.32
129 SER OG	31.11	18.56	6.62	14.12
129 SER C	30.68	20.52	4.37	9.06
129 SER O	29.51	20.77	4.20	11.11
130 LEU N	31.47	20.13	3.38	8.54
130 LEU CA	30.93	19.85	2.07	8.69
130 LEU CB	31.97	20.16	0.99	12.13
130 LEU CG	31.88	19.67	-0.47	11.59
130 LEU CD1	30.63	20.19	-1.18	7.88
130 LEU CD2	33.15	20.15	-1.20	12.99
130 LEU C	30.56	18.41	1.96	7.67
130 LEU O	31.36	17.56	2.22	10.85
131 SER N	29.32	18.10	1.66	7.41

Fig. 3C

Residue Atom	X	Y	Z	B
131 SER CA	29.03	16.71	1.46	10.24
131 SER CB	27.65	16.35	1.96	12.02
131 SER OG	27.68	16.30	3.36	18.85
131 SER C	29.16	16.49	-0.04	12.33
131 SER O	28.84	17.37	-0.85	13.24
132 THR N	29.73	15.36	-0.41	14.15
132 THR CA	29.89	14.98	-1.80	15.87
132 THR CB	31.34	14.59	-2.10	13.37
132 THR OG1	31.80	13.73	-1.08	12.74
132 THR CG2	32.24	15.82	-2.18	11.44
132 THR C	29.00	13.77	-1.94	18.29
132 THR O	29.23	12.74	-1.28	19.88
148 HIS N	25.72	18.90	-0.80	8.71
148 HIS CA	25.34	20.14	-0.15	8.60
148 HIS C	26.51	20.61	0.73	8.75
148 HIS O	27.57	20.01	0.73	9.64
148 HIS CB	24.11	19.91	0.72	7.49
148 HIS CG	24.35	18.95	1.85	10.55
148 HIS ND1	24.75	19.32	3.11	14.28
148 HIS CD2	24.25	17.60	1.89	13.72
148 HIS NE2	24.59	17.13	3.17	10.96
148 HIS CE1	24.88	18.20	3.87	11.30
149 VAL N	26.28	21.66	1.52	5.64
149 VAL CA	27.28	22.20	2.42	4.43
149 VAL CB	27.91	23.52	1.85	2.00
149 VAL CG1	27.13	24.01	0.72	2.60
149 VAL CG2	28.02	24.63	2.90	2.00
149 VAL C	26.66	22.41	3.81	5.08
149 VAL O	25.76	23.23	3.99	6.81
150 ALA N	27.07	21.63	4.79	4.31
150 ALA CA	26.54	21.77	6.12	4.19

Fig. 3D

Residue Atom	X	Y	Z	B
150 ALA CB	26.61	20.47	6.82	2.00
150 ALA C	27.27	22.85	6.92	6.21
150 ALA O	28.45	23.04	6.74	8.36
151 LEU N	26.52	23.64	7.70	8.89
151 LEU CA	27.04	24.68	8.59	8.16
151 LEU CB	25.96	25.72	8.87	6.76
151 LEU CG	26.17	27.20	8.57	13.35
151 LEU CD1	26.80	27.33	7.16	14.96
151 LEU CD2	24.86	28.01	8.69	2.52
151 LEU C	27.28	23.87	9.88	10.36
151 LEU O	26.40	23.13	10.32	11.10
152 CYS N	28.45	23.97	10.47	10.07
152 CYS CA	28.70	23.20	11.68	10.06
152 CYS CB	29.09	21.78	11.30	9.56
152 CYS SG	30.55	21.68	10.32	12.05
152 CYS C	29.70	23.84	12.62	10.73
152 CYS O	30.22	24.91	12.35	10.79
154 ILE N	32.67	22.27	14.19	13.17
154 ILE CA	34.04	21.91	13.84	14.44
154 ILE CB	34.76	21.20	15.06	16.21
154 ILE CG2	35.94	20.37	14.62	16.07
154 ILE CG1	35.25	22.26	16.04	18.38
154 ILE CD1	36.24	23.28	15.42	19.24
154 ILE C	33.90	20.99	12.62	14.39
154 ILE O	33.23	19.97	12.69	13.58
155 GLY N	34.40	21.47	11.48	16.35
155 GLY CA	34.31	20.72	10.24	18.21
155 GLY C	35.41	19.67	10.20	20.38
155 GLY O	36.41	19.78	10.93	21.76
156 ARG N	35.26	18.69	9.32	20.77
156 ARG CA	36.24	17.61	9.21	21.11

Fig. 3E

Residue	Atom	X	Y	Z	B
156 ARG	CB	35.53	16.30	8.87	24.90
156 ARG	CG	35.76	15.25	9.94	29.04
156 ARG	CD	34.71	14.16	9.85	32.89
156 ARG	NE	34.84	13.39	8.62	39.65
156 ARG	CZ	34.67	12.06	8.54	43.91
156 ARG	NH1	34.81	11.44	7.34	44.98
156 ARG	NH2	34.32	11.35	9.63	42.89
156 ARG	C	37.40	17.83	8.24	20.04
156 ARG	O	38.31	17.01	8.18	22.30
157 ARG	N	37.35	18.89	7.45	17.53
157 ARG	CA	38.43	19.17	6.53	15.10
157 ARG	CB	37.95	19.20	5.08	11.19
157 ARG	CG	37.67	17.82	4.59	7.60
157 ARG	CD	37.61	17.73	3.11	10.17
157 ARG	NE	36.33	18.14	2.57	15.38
157 ARG	CZ	35.39	17.30	2.14	17.80
157 ARG	NH1	35.56	15.99	2.20	14.74
157 ARG	NH2	34.30	17.77	1.53	18.94
157 ARG	C	39.11	20.45	7.00	15.95
157 ARG	O	38.48	21.29	7.67	15.82
321 WAT	OH2	34.16	20.32	7.14	15.58

Fig. 4A

ATOM	1	CB	ALA	A	17	10.980	40.209	8.106	1.00	31.97
ATOM	2	C	ALA	A	17	13.480	40.173	8.007	1.00	27.25
ATOM	3	O	ALA	A	17	14.076	40.347	9.079	1.00	26.95
ATOM	4	N	ALA	A	17	12.141	41.223	6.151	1.00	26.54
ATOM	5	CA	ALA	A	17	12.217	40.962	7.629	1.00	28.53
ATOM	6	N	ALA	A	18	13.850	39.255	7.120	1.00	27.32
ATOM	7	CA	ALA	A	18	15.059	38.441	7.337	1.00	25.64
ATOM	8	CB	ALA	A	18	15.030	37.202	6.471	1.00	23.07
ATOM	9	C	ALA	A	18	16.260	39.306	6.980	1.00	22.24
ATOM	10	O	ALA	A	18	16.185	40.221	6.154	1.00	21.42
ATOM	11	N	VAL	A	19	17.343	39.069	7.711	1.00	22.87
ATOM	12	CA	VAL	A	19	18.635	39.758	7.485	1.00	16.87
ATOM	13	CB	VAL	A	19	19.447	39.903	8.801	1.00	17.31
ATOM	14	CG1	VAL	A	19	20.873	40.382	8.529	1.00	16.47
ATOM	15	CG2	VAL	A	19	18.773	40.870	9.711	1.00	17.73
ATOM	16	C	VAL	A	19	19.349	38.757	6.565	1.00	12.56
ATOM	17	O	VAL	A	19	19.512	37.578	6.888	1.00	13.32
ATOM	18	N	PRO	A	20	19.629	39.176	5.333	1.00	9.51
ATOM	19	CD	PRO	A	20	19.146	40.372	4.636	1.00	7.49
ATOM	20	CA	PRO	A	20	20.318	38.269	4.413	1.00	7.09
ATOM	21	CB	PRO	A	20	20.239	39.011	3.078	1.00	10.46
ATOM	22	CG	PRO	A	20	19.018	39.861	3.222	1.00	9.68
ATOM	23	C	PRO	A	20	21.742	38.196	4.897	1.00	6.66
ATOM	24	O	PRO	A	20	22.429	39.197	5.037	1.00	12.21
ATOM	25	N	ILE	A	21	22.183	36.996	5.191	1.00	6.42
ATOM	26	CA	ILE	A	21	23.537	36.791	5.683	1.00	6.75
ATOM	27	CB	ILE	A	21	23.481	35.922	6.984	1.00	9.36
ATOM	28	CG2	ILE	A	21	24.860	35.410	7.387	1.00	8.42
ATOM	29	CG1	ILE	A	21	22.848	36.713	8.126	1.00	7.06
ATOM	30	CD1	ILE	A	21	22.600	35.873	9.373	1.00	9.87
ATOM	31	C	ILE	A	21	24.342	36.056	4.610	1.00	7.41
ATOM	32	O	ILE	A	21	23.852	35.129	3.976	1.00	7.22
ATOM	33	N	TYR	A	22	25.567	36.522	4.376	1.00	10.46
ATOM	34	CA	TYR	A	22	26.522	35.876	3.420	1.00	8.42
ATOM	35	CB	TYR	A	22	27.248	36.920	2.597	1.00	9.47
ATOM	36	CG	TYR	A	22	26.318	37.634	1.718	1.00	11.88
ATOM	37	CD1	TYR	A	22	26.025	37.134	0.460	1.00	16.31
ATOM	38	CE1	TYR	A	22	25.084	37.734	-0.340	1.00	16.44
ATOM	39	CD2	TYR	A	22	25.653	38.764	2.156	1.00	11.71
ATOM	40	CE2	TYR	A	22	24.710	39.377	1.361	1.00	11.64
ATOM	41	CZ	TYR	A	22	24.431	38.851	0.119	1.00	16.41
ATOM	42	OH	TYR	A	22	23.476	39.422	-0.671	1.00	24.08
ATOM	43	C	TYR	A	22	27.561	35.060	4.232	1.00	8.38
ATOM	44	O	TYR	A	22	28.061	35.486	5.281	1.00	6.96
ATOM	45	N	VAL	A	23	27.838	33.857	3.747	1.00	7.92
ATOM	46	CA	VAL	A	23	28.829	32.966	4.376	1.00	7.55
ATOM	47	CB	VAL	A	23	28.298	31.531	4.564	1.00	7.21
ATOM	48	CG1	VAL	A	23	28.894	30.874	5.794	1.00	2.00
ATOM	49	CG2	VAL	A	23	26.832	31.508	4.557	1.00	5.18
ATOM	50	C	VAL	A	23	29.868	32.854	3.260	1.00	8.10
ATOM	51	O	VAL	A	23	29.536	32.829	2.080	1.00	12.46

Fig. 4B

ATOM	52	N	ALA	A	24	31.125	32.733	3.627	1.00	5.41
ATOM	53	CA	ALA	A	24	32.187	32.593	2.627	1.00	2.87
ATOM	54	CB	ALA	A	24	32.712	33.965	2.229	1.00	2.00
ATOM	55	C	ALA	A	24	33.250	31.799	3.351	1.00	6.88
ATOM	56	O	ALA	A	24	33.368	31.890	4.573	1.00	10.26
ATOM	57	N	GLY	A	25	33.970	30.952	2.622	1.00	7.52
ATOM	58	CA	GLY	A	25	35.015	30.159	3.234	1.00	2.00
ATOM	59	C	GLY	A	25	35.416	29.067	2.288	1.00	5.06
ATOM	60	O	GLY	A	25	34.807	28.898	1.236	1.00	8.24
ATOM	61	N	PHE	A	26	36.463	28.340	2.643	1.00	8.52
ATOM	62	CA	PHE	A	26	36.950	27.220	1.810	1.00	6.14
ATOM	63	CB	PHE	A	26	38.474	26.990	1.985	1.00	3.33
ATOM	64	CG	PHE	A	26	39.347	27.965	1.206	1.00	6.92
ATOM	65	CD1	PHE	A	26	39.879	29.107	1.818	1.00	8.24
ATOM	66	CD2	PHE	A	26	39.665	27.727	-0.132	1.00	6.96
ATOM	67	CE1	PHE	A	26	40.711	29.984	1.102	1.00	4.75
ATOM	68	CE2	PHE	A	26	40.502	28.603	-0.856	1.00	3.94
ATOM	69	CZ	PHE	A	26	41.021	29.725	-0.239	1.00	2.00
ATOM	70	C	PHE	A	26	36.168	25.973	2.222	1.00	4.85
ATOM	71	O	PHE	A	26	35.893	25.704	3.398	1.00	3.88
ATOM	72	N	LEU	A	27	35.736	25.246	1.206	1.00	5.10
ATOM	73	CA	LEU	A	27	35.022	24.000	1.421	1.00	6.35
ATOM	74	CB	LEU	A	27	34.241	23.628	0.173	1.00	4.80
ATOM	75	CG	LEU	A	27	32.753	23.867	0.051	1.00	2.00
ATOM	76	CD1	LEU	A	27	32.147	24.549	1.270	1.00	2.00
ATOM	77	CD2	LEU	A	27	32.558	24.628	-1.224	1.00	2.00
ATOM	78	C	LEU	A	27	36.089	22.929	1.732	1.00	8.64
ATOM	79	O	LEU	A	27	35.816	21.898	2.340	1.00	8.93
ATOM	80	N	ALA	A	28	37.308	23.191	1.258	1.00	9.18
ATOM	81	CA	ALA	A	28	38.464	22.295	1.443	1.00	6.84
ATOM	82	CB	ALA	A	28	38.247	21.026	0.660	1.00	8.67
ATOM	83	C	ALA	A	28	39.763	22.986	0.965	1.00	9.42
ATOM	84	O	ALA	A	28	39.751	23.869	0.111	1.00	10.30
ATOM	85	N	LEU	A	29	40.888	22.591	1.561	1.00	11.25
ATOM	86	CA	LEU	A	29	42.226	23.138	1.173	1.00	12.15
ATOM	87	CB	LEU	A	29	43.035	23.608	2.388	1.00	10.90
ATOM	88	CG	LEU	A	29	42.517	24.776	3.233	1.00	6.47
ATOM	89	CD1	LEU	A	29	43.379	24.840	4.442	1.00	7.44
ATOM	90	CD2	LEU	A	29	42.530	26.106	2.498	1.00	2.00
ATOM	91	C	LEU	A	29	42.912	21.952	0.486	1.00	12.45
ATOM	92	O	LEU	A	29	42.949	20.854	1.018	1.00	14.70
ATOM	93	N	TYR	A	30	43.431	22.201	-0.714	1.00	15.16
ATOM	94	CA	TYR	A	30	44.080	21.186	-1.553	1.00	17.04
ATOM	95	CB	TYR	A	30	44.473	21.823	-2.867	1.00	12.21
ATOM	96	CG	TYR	A	30	43.306	22.048	-3.780	1.00	12.98
ATOM	97	CD1	TYR	A	30	42.289	21.099	-3.881	1.00	3.60
ATOM	98	CE1	TYR	A	30	41.240	21.308	-4.746	1.00	4.61
ATOM	99	CD2	TYR	A	30	43.227	23.203	-4.571	1.00	7.48
ATOM	100	CE2	TYR	A	30	42.180	23.409	-5.429	1.00	2.00
ATOM	101	CZ	TYR	A	30	41.199	22.464	-5.511	1.00	2.00
ATOM	102	OH	TYR	A	30	40.166	22.662	-6.376	1.00	7.18
ATOM	103	C	TYR	A	30	45.239	20.315	-1.021	1.00	23.99

Fig. 4C

ATOM	104	O	TYR	A	30	45.216	19.081	-1.157	1.00	35.15
ATOM	105	N	ASP	A	31	46.284	20.906	-0.466	1.00	16.90
ATOM	106	CA	ASP	A	31	47.369	20.015	0.028	1.00	21.03
ATOM	107	CB	ASP	A	31	48.678	20.216	-0.769	1.00	24.41
ATOM	108	CG	ASP	A	31	48.693	19.462	-2.114	1.00	27.07
ATOM	109	OD1	ASP	A	31	48.911	20.097	-3.178	1.00	33.82
ATOM	110	OD2	ASP	A	31	48.517	18.225	-2.118	1.00	27.94
ATOM	111	C	ASP	A	31	47.526	20.346	1.494	1.00	23.37
ATOM	112	O	ASP	A	31	48.559	20.829	1.955	1.00	26.14
ATOM	113	N	SER	A	32	46.439	20.089	2.223	1.00	22.26
ATOM	114	CA	SER	A	32	46.348	20.395	3.687	1.00	24.96
ATOM	115	CB	SER	A	32	44.953	20.963	4.013	1.00	23.87
ATOM	116	OG	SER	A	32	43.933	20.112	3.521	1.00	22.56
ATOM	117	C	SER	A	32	46.691	19.255	4.664	1.00	23.19
ATOM	118	O	SER	A	32	47.031	19.464	5.830	1.00	24.17
ATOM	119	N	GLY	A	33	46.560	18.034	4.172	1.00	21.42
ATOM	120	CA	GLY	A	33	46.845	16.892	4.999	1.00	17.05
ATOM	121	C	GLY	A	33	45.571	16.203	5.409	1.00	20.62
ATOM	122	O	GLY	A	33	45.594	15.459	6.377	1.00	24.68
ATOM	123	N	ASP	A	34	44.455	16.464	4.720	1.00	22.48
ATOM	124	CA	ASP	A	34	43.133	15.793	5.068	1.00	22.57
ATOM	125	CB	ASP	A	34	41.981	16.214	4.126	1.00	17.56
ATOM	126	CG	ASP	A	34	41.390	17.572	4.455	1.00	12.57
ATOM	127	OD1	ASP	A	34	41.118	18.353	3.519	1.00	17.61
ATOM	128	OD2	ASP	A	34	41.161	17.858	5.633	1.00	10.35
ATOM	129	C	ASP	A	34	43.359	14.276	4.937	1.00	24.91
ATOM	130	O	ASP	A	34	44.117	13.803	4.085	1.00	29.90
ATOM	131	N	PRO	A	35	42.703	13.490	5.795	1.00	25.20
ATOM	132	CD	PRO	A	35	41.853	13.864	6.936	1.00	26.67
ATOM	133	CA	PRO	A	35	42.879	12.038	5.716	1.00	26.21
ATOM	134	CB	PRO	A	35	41.850	11.527	6.707	1.00	26.43
ATOM	135	CG	PRO	A	35	41.881	12.607	7.768	1.00	28.24
ATOM	136	C	PRO	A	35	42.618	11.527	4.290	1.00	29.80
ATOM	137	O	PRO	A	35	42.139	12.248	3.420	1.00	29.68
ATOM	138	N	GLY	A	36	42.921	10.252	4.067	1.00	35.36
ATOM	139	CA	GLY	A	36	42.755	9.668	2.744	1.00	33.76
ATOM	140	C	GLY	A	36	41.429	9.970	2.100	1.00	34.27
ATOM	141	O	GLY	A	36	41.359	10.597	1.054	1.00	32.21
ATOM	142	N	GLU	A	37	40.369	9.560	2.778	1.00	36.66
ATOM	143	CA	GLU	A	37	38.991	9.746	2.289	1.00	37.10
ATOM	144	CB	GLU	A	37	38.037	9.040	3.274	1.00	48.49
ATOM	145	CG	GLU	A	37	36.527	9.343	3.059	1.00	55.75
ATOM	146	CD	GLU	A	37	35.613	8.655	4.068	1.00	57.77
ATOM	147	OE1	GLU	A	37	35.672	8.990	5.277	1.00	59.61
ATOM	148	OE2	GLU	A	37	34.823	7.787	3.635	1.00	60.72
ATOM	149	C	GLU	A	37	38.515	11.192	2.013	1.00	33.55
ATOM	150	O	GLU	A	37	37.959	11.515	0.969	1.00	37.68
ATOM	151	N	LEU	A	38	38.679	12.044	3.012	1.00	26.85
ATOM	152	CA	LEU	A	38	38.221	13.442	2.935	1.00	20.79
ATOM	153	CB	LEU	A	38	38.298	14.040	4.341	1.00	19.20
ATOM	154	CG	LEU	A	38	37.385	13.373	5.387	1.00	19.62
ATOM	155	CD1	LEU	A	38	37.541	14.052	6.749	1.00	14.44

Fig. 4D

ATOM	156	CD2	LEU	A	38	35.921	13.404	4.918	1.00	12.06
ATOM	157	C	LEU	A	38	38.902	14.349	1.898	1.00	18.61
ATOM	158	O	LEU	A	38	38.318	15.277	1.372	1.00	19.33
ATOM	159	N	ALA	A	39	40.167	14.077	1.631	1.00	18.81
ATOM	160	CA	ALA	A	39	40.970	14.880	0.683	1.00	20.42
ATOM	161	CB	ALA	A	39	42.280	14.175	0.393	1.00	21.73
ATOM	162	C	ALA	A	39	40.269	15.208	-0.632	1.00	21.36
ATOM	163	O	ALA	A	39	39.540	14.416	-1.217	1.00	26.23
ATOM	164	N	LEU	A	40	40.547	16.408	-1.118	1.00	20.60
ATOM	165	CA	LEU	A	40	39.977	16.891	-2.390	1.00	17.27
ATOM	166	CB	LEU	A	40	38.922	17.964	-2.130	1.00	21.23
ATOM	167	CG	LEU	A	40	37.489	17.482	-1.898	1.00	20.88
ATOM	168	CD1	LEU	A	40	36.603	18.647	-1.462	1.00	21.76
ATOM	169	CD2	LEU	A	40	36.960	16.857	-3.167	1.00	15.74
ATOM	170	C	LEU	A	40	41.136	17.452	-3.189	1.00	13.74
ATOM	171	O	LEU	A	40	42.063	18.035	-2.644	1.00	14.61
ATOM	172	N	ASP	A	41	41.071	17.284	-4.501	1.00	12.75
ATOM	173	CA	ASP	A	41	42.139	17.763	-5.377	1.00	11.19
ATOM	174	CB	ASP	A	41	42.921	16.572	-5.885	1.00	13.80
ATOM	175	CG	ASP	A	41	42.080	15.650	-6.682	1.00	15.44
ATOM	176	OD1	ASP	A	41	42.092	15.759	-7.933	1.00	19.46
ATOM	177	OD2	ASP	A	41	41.407	14.826	-6.044	1.00	16.75
ATOM	178	C	ASP	A	41	41.600	18.629	-6.517	1.00	8.12
ATOM	179	O	ASP	A	41	40.440	18.583	-6.865	1.00	11.10
ATOM	180	N	PRO	A	42	42.486	19.394	-7.169	1.00	9.16
ATOM	181	CD	PRO	A	42	43.932	19.509	-6.923	1.00	2.03
ATOM	182	CA	PRO	A	42	42.101	20.283	-8.266	1.00	6.51
ATOM	183	CB	PRO	A	42	43.436	20.806	-8.751	1.00	2.00
ATOM	184	CG	PRO	A	42	44.224	20.841	-7.562	1.00	2.00
ATOM	185	C	PRO	A	42	41.296	19.677	-9.394	1.00	8.97
ATOM	186	O	PRO	A	42	40.256	20.180	-9.796	1.00	8.38
ATOM	187	N	ASP	A	43	41.767	18.561	-9.914	1.00	9.69
ATOM	188	CA	ASP	A	43	41.033	17.943	-11.015	1.00	12.54
ATOM	189	CB	ASP	A	43	41.862	16.838	-11.622	1.00	17.14
ATOM	190	CG	ASP	A	43	42.792	17.345	-12.685	1.00	23.39
ATOM	191	OD1	ASP	A	43	42.591	18.464	-13.198	1.00	25.32
ATOM	192	OD2	ASP	A	43	43.730	16.610	-13.019	1.00	29.45
ATOM	193	C	ASP	A	43	39.627	17.457	-10.650	1.00	11.48
ATOM	194	O	ASP	A	43	38.710	17.553	-11.436	1.00	13.95
ATOM	195	N	THR	A	44	39.464	16.910	-9.451	1.00	12.99
ATOM	196	CA	THR	A	44	38.132	16.450	-9.012	1.00	12.32
ATOM	197	CB	THR	A	44	38.235	15.592	-7.784	1.00	10.64
ATOM	198	OG1	THR	A	44	39.153	14.540	-8.072	1.00	4.70
ATOM	199	CG2	THR	A	44	36.885	14.972	-7.445	1.00	16.51
ATOM	200	C	THR	A	44	37.194	17.639	-8.756	1.00	13.28
ATOM	201	O	THR	A	44	35.981	17.565	-8.938	1.00	13.50
ATOM	202	N	VAL	A	45	37.768	18.764	-8.352	1.00	7.49
ATOM	203	CA	VAL	A	45	36.919	19.905	-8.134	1.00	7.31
ATOM	204	CB	VAL	A	45	37.571	20.941	-7.270	1.00	5.44
ATOM	205	CG1	VAL	A	45	36.684	22.165	-7.172	1.00	3.80
ATOM	206	CG2	VAL	A	45	37.772	20.364	-5.888	1.00	8.22
ATOM	207	C	VAL	A	45	36.555	20.480	-9.488	1.00	11.60

Fig. 4E

ATOM	208	O	VAL	A	45	35.413	20.840	-9.756	1.00	19.59
ATOM	209	N	ARG	A	46	37.529	20.488	-10.380	1.00	11.14
ATOM	210	CA	ARG	A	46	37.337	21.025	-11.734	1.00	13.59
ATOM	211	CB	ARG	A	46	38.594	20.804	-12.562	1.00	19.57
ATOM	212	CG	ARG	A	46	38.741	21.707	-13.777	1.00	32.87
ATOM	213	CD	ARG	A	46	39.159	23.150	-13.381	1.00	51.39
ATOM	214	NE	ARG	A	46	38.054	23.942	-12.791	1.00	61.85
ATOM	215	CZ	ARG	A	46	38.090	25.255	-12.512	1.00	60.50
ATOM	216	NH1	ARG	A	46	37.009	25.837	-11.986	1.00	58.23
ATOM	217	NH2	ARG	A	46	39.181	25.988	-12.751	1.00	57.75
ATOM	218	C	ARG	A	46	36.153	20.334	-12.386	1.00	11.46
ATOM	219	O	ARG	A	46	35.281	20.936	-12.971	1.00	14.55
ATOM	220	N	ALA	A	47	36.112	19.026	-12.224	1.00	9.86
ATOM	221	CA	ALA	A	47	35.048	18.202	-12.812	1.00	9.60
ATOM	222	CB	ALA	A	47	35.499	16.765	-12.814	1.00	2.00
ATOM	223	C	ALA	A	47	33.658	18.329	-12.115	1.00	8.75
ATOM	224	O	ALA	A	47	32.653	17.857	-12.604	1.00	10.75
ATOM	225	N	ALA	A	48	33.619	18.961	-10.955	1.00	10.20
ATOM	226	CA	ALA	A	48	32.363	19.098	-10.221	1.00	8.04
ATOM	227	CB	ALA	A	48	32.610	18.863	-8.761	1.00	2.69
ATOM	228	C	ALA	A	48	31.737	20.470	-10.438	1.00	11.37
ATOM	229	O	ALA	A	48	30.618	20.739	-10.032	1.00	14.85
ATOM	230	N	LEU	A	49	32.465	21.346	-11.112	1.00	11.13
ATOM	231	CA	LEU	A	49	31.979	22.703	-11.330	1.00	11.79
ATOM	232	CB	LEU	A	49	33.047	23.684	-10.857	1.00	12.92
ATOM	233	CG	LEU	A	49	33.663	23.406	-9.481	1.00	15.46
ATOM	234	CD1	LEU	A	49	34.707	24.462	-9.188	1.00	9.31
ATOM	235	CD2	LEU	A	49	32.595	23.352	-8.384	1.00	10.40
ATOM	236	C	LEU	A	49	31.571	22.981	-12.780	1.00	19.21
ATOM	237	O	LEU	A	49	32.261	22.618	-13.723	1.00	19.07
ATOM	238	N	PRO	A	50	30.412	23.635	-12.978	1.00	23.72
ATOM	239	CD	PRO	A	50	30.023	24.107	-14.310	1.00	24.14
ATOM	240	CA	PRO	A	50	29.454	24.124	-11.978	1.00	23.03
ATOM	241	CB	PRO	A	50	28.536	25.039	-12.789	1.00	23.46
ATOM	242	CG	PRO	A	50	29.352	25.399	-13.972	1.00	27.62
ATOM	243	C	PRO	A	50	28.652	22.958	-11.459	1.00	18.14
ATOM	244	O	PRO	A	50	28.526	21.931	-12.109	1.00	18.10
ATOM	245	N	PRO	A	51	28.099	23.104	-10.254	1.00	18.73
ATOM	246	CD	PRO	A	51	28.320	24.148	-9.234	1.00	18.25
ATOM	247	CA	PRO	A	51	27.313	21.994	-9.723	1.00	20.17
ATOM	248	CB	PRO	A	51	26.927	22.495	-8.333	1.00	19.76
ATOM	249	CG	PRO	A	51	28.104	23.388	-7.961	1.00	19.37
ATOM	250	C	PRO	A	51	26.083	21.738	-10.613	1.00	18.98
ATOM	251	O	PRO	A	51	25.473	22.650	-11.142	1.00	17.43
ATOM	252	N	GLU	A	52	25.769	20.469	-10.825	1.00	20.72
ATOM	253	CA	GLU	A	52	24.592	20.102	-11.633	1.00	27.18
ATOM	254	CB	GLU	A	52	24.444	18.587	-11.623	1.00	30.68
ATOM	255	CG	GLU	A	52	23.234	18.060	-12.376	1.00	38.66
ATOM	256	CD	GLU	A	52	23.353	18.247	-13.863	1.00	43.25
ATOM	257	OE1	GLU	A	52	22.803	19.243	-14.377	1.00	47.66
ATOM	258	OE2	GLU	A	52	23.997	17.396	-14.514	1.00	47.58
ATOM	259	C	GLU	A	52	23.342	20.798	-11.011	1.00	28.46

Fig. 4F

ATOM	260	O	GLU	A	52	22.564	21.519	-11.646	1.00	25.49
ATOM	261	N	ASN	A	53	23.188	20.580	-9.714	1.00	31.10
ATOM	262	CA	ASN	A	53	22.067	21.176	-8.981	1.00	33.66
ATOM	263	CB	ASN	A	53	21.158	20.075	-8.436	1.00	40.90
ATOM	264	CG	ASN	A	53	20.249	19.494	-9.510	1.00	48.10
ATOM	265	OD1	ASN	A	53	20.377	18.327	-9.871	1.00	54.90
ATOM	266	ND2	ASN	A	53	19.332	20.312	-10.035	1.00	49.48
ATOM	267	C	ASN	A	53	22.564	22.109	-7.878	1.00	29.61
ATOM	268	O	ASN	A	53	23.666	21.951	-7.359	1.00	32.75
ATOM	269	N	PRO	A	54	21.752	23.122	-7.527	1.00	26.65
ATOM	270	CD	PRO	A	54	20.408	23.409	-8.062	1.00	30.19
ATOM	271	CA	PRO	A	54	22.097	24.095	-6.491	1.00	22.46
ATOM	272	CB	PRO	A	54	20.815	24.914	-6.345	1.00	29.07
ATOM	273	CG	PRO	A	54	20.239	24.878	-7.731	1.00	33.83
ATOM	274	C	PRO	A	54	22.450	23.408	-5.199	1.00	15.80
ATOM	275	O	PRO	A	54	21.956	22.341	-4.858	1.00	14.86
ATOM	276	N	LEU	A	55	23.370	24.024	-4.484	1.00	12.78
ATOM	277	CA	LEU	A	55	23.783	23.460	-3.231	1.00	5.47
ATOM	278	CB	LEU	A	55	25.284	23.570	-3.036	1.00	7.35
ATOM	279	CG	LEU	A	55	26.122	22.704	-3.957	1.00	8.64
ATOM	280	CD1	LEU	A	55	27.572	22.922	-3.657	1.00	15.60
ATOM	281	CD2	LEU	A	55	25.768	21.275	-3.725	1.00	10.92
ATOM	282	C	LEU	A	55	23.060	24.199	-2.157	1.00	5.03
ATOM	283	O	LEU	A	55	23.183	25.399	-2.004	1.00	11.73
ATOM	284	N	PRO	A	56	22.155	23.512	-1.485	1.00	4.24
ATOM	285	CD	PRO	A	56	21.635	22.179	-1.824	1.00	2.00
ATOM	286	CA	PRO	A	56	21.394	24.111	-0.394	1.00	3.54
ATOM	287	CB	PRO	A	56	20.343	23.050	-0.122	1.00	4.57
ATOM	288	CG	PRO	A	56	21.025	21.780	-0.547	1.00	2.00
ATOM	289	C	PRO	A	56	22.337	24.217	0.818	1.00	4.48
ATOM	290	O	PRO	A	56	23.371	23.542	0.875	1.00	6.64
ATOM	291	N	ILE	A	57	21.995	25.068	1.782	1.00	2.94
ATOM	292	CA	ILE	A	57	22.823	25.182	2.991	1.00	2.00
ATOM	293	CB	ILE	A	57	23.305	26.620	3.252	1.00	4.36
ATOM	294	CG2	ILE	A	57	23.900	26.738	4.695	1.00	2.00
ATOM	295	CG1	ILE	A	57	24.299	27.056	2.172	1.00	2.00
ATOM	296	CD1	ILE	A	57	24.677	28.481	2.269	1.00	2.00
ATOM	297	C	ILE	A	57	21.926	24.775	4.139	1.00	4.15
ATOM	298	O	ILE	A	57	20.816	25.275	4.294	1.00	3.38
ATOM	299	N	ASN	A	58	22.372	23.796	4.906	1.00	4.69
ATOM	300	CA	ASN	A	58	21.591	23.377	6.049	1.00	7.45
ATOM	301	CB	ASN	A	58	20.933	22.038	5.793	1.00	11.69
ATOM	302	CG	ASN	A	58	21.882	21.008	5.311	1.00	15.54
ATOM	303	OD1	ASN	A	58	22.949	20.827	5.869	1.00	22.74
ATOM	304	ND2	ASN	A	58	21.480	20.277	4.285	1.00	24.85
ATOM	305	C	ASN	A	58	22.423	23.393	7.327	1.00	10.45
ATOM	306	O	ASN	A	58	23.607	23.670	7.298	1.00	9.69
ATOM	307	N	VAL	A	59	21.766	23.203	8.470	1.00	11.45
ATOM	308	CA	VAL	A	59	22.467	23.226	9.764	1.00	9.16
ATOM	309	CB	VAL	A	59	21.639	23.911	10.870	1.00	8.10
ATOM	310	CG1	VAL	A	59	22.366	23.801	12.195	1.00	8.74
ATOM	311	CG2	VAL	A	59	21.415	25.376	10.544	1.00	3.69

Fig. 4G

ATOM	312	C	VAL	A	59	22.786	21.821	10.211	1.00	13.11
ATOM	313	O	VAL	A	59	21.932	20.957	10.268	1.00	15.12
ATOM	314	N	ASP	A	60	24.054	21.586	10.505	1.00	20.34
ATOM	315	CA	ASP	A	60	24.514	20.256	10.991	1.00	32.81
ATOM	316	CB	ASP	A	60	24.285	20.194	12.514	1.00	40.06
ATOM	317	CG	ASP	A	60	25.230	19.225	13.226	1.00	46.11
ATOM	318	OD1	ASP	A	60	26.474	19.401	13.129	1.00	48.62
ATOM	319	OD2	ASP	A	60	24.718	18.292	13.900	1.00	50.43
ATOM	320	C	ASP	A	60	23.866	19.032	10.254	1.00	36.61
ATOM	321	O	ASP	A	60	23.201	18.163	10.839	1.00	39.35
ATOM	322	N	HIS	A	61	24.053	19.024	8.937	1.00	41.05
ATOM	323	CA	HIS	A	61	23.564	17.952	8.013	1.00	47.22
ATOM	324	CB	HIS	A	61	24.547	16.770	7.982	1.00	47.84
ATOM	325	CG	HIS	A	61	25.792	17.052	7.195	1.00	49.75
ATOM	326	CD2	HIS	A	61	25.965	17.423	5.907	1.00	51.27
ATOM	327	ND1	HIS	A	61	27.049	17.028	7.757	1.00	51.98
ATOM	328	CE1	HIS	A	61	27.943	17.377	6.847	1.00	53.59
ATOM	329	NE2	HIS	A	61	27.311	17.623	5.713	1.00	50.47
ATOM	330	C	HIS	A	61	22.126	17.445	8.142	1.00	49.08
ATOM	331	O	HIS	A	61	21.680	16.560	7.392	1.00	53.07
ATOM	332	N	ARG	A	62	21.406	18.012	9.103	1.00	47.98
ATOM	333	CA	ARG	A	62	20.002	17.686	9.322	1.00	45.13
ATOM	334	CB	ARG	A	62	19.558	18.379	10.602	1.00	48.49
ATOM	335	CG	ARG	A	62	19.694	17.540	11.869	1.00	56.34
ATOM	336	CD	ARG	A	62	18.561	16.509	11.937	1.00	63.51
ATOM	337	NE	ARG	A	62	17.279	17.081	11.504	1.00	67.20
ATOM	338	CZ	ARG	A	62	16.272	17.389	12.317	1.00	67.07
ATOM	339	NH1	ARG	A	62	16.383	17.174	13.628	1.00	67.89
ATOM	340	NH2	ARG	A	62	15.162	17.928	11.815	1.00	65.00
ATOM	341	C	ARG	A	62	19.353	18.305	8.061	1.00	42.93
ATOM	342	O	ARG	A	62	19.083	19.513	8.001	1.00	42.60
ATOM	343	N	ALA	A	63	19.193	17.481	7.023	1.00	40.84
ATOM	344	CA	ALA	A	63	18.627	17.948	5.721	1.00	40.08
ATOM	345	CB	ALA	A	63	18.606	16.822	4.702	1.00	36.71
ATOM	346	C	ALA	A	63	17.250	18.651	5.785	1.00	42.68
ATOM	347	O	ALA	A	63	16.783	19.234	4.812	1.00	42.31
ATOM	348	N	ARG	A	64	16.588	18.554	6.938	1.00	44.53
ATOM	349	CA	ARG	A	64	15.249	19.240	7.162	1.00	45.15
ATOM	350	CB	ARG	A	64	14.541	18.716	8.425	1.00	52.01
ATOM	351	CG	ARG	A	64	14.178	17.223	8.388	1.00	61.80
ATOM	352	CD	ARG	A	64	12.681	17.016	8.169	1.00	68.05
ATOM	353	NE	ARG	A	64	12.006	16.573	9.388	1.00	75.79
ATOM	354	CZ	ARG	A	64	11.603	15.328	9.663	1.00	79.65
ATOM	355	NH1	ARG	A	64	11.789	14.319	8.810	1.00	80.90
ATOM	356	NH2	ARG	A	64	10.986	15.097	10.815	1.00	79.73
ATOM	357	C	ARG	A	64	15.510	20.745	7.362	1.00	38.34
ATOM	358	O	ARG	A	64	14.659	21.607	7.042	1.00	40.42
ATOM	359	N	CYS	A	65	16.723	21.034	7.856	1.00	26.96
ATOM	360	CA	CYS	A	65	17.169	22.412	8.179	1.00	20.44
ATOM	361	CB	CYS	A	65	18.129	22.373	9.329	1.00	18.01
ATOM	362	SG	CYS	A	65	17.322	22.682	10.775	1.00	22.41
ATOM	363	C	CYS	A	65	17.789	23.225	7.090	1.00	15.86

Fig. 4H

ATOM	364	O	CYS A	65	18.883	23.742	7.234	1.00	19.52
ATOM	365	N	GLU A	66	17.071	23.404	6.007	1.00	9.13
ATOM	366	CA	GLU A	66	17.605	24.185	4.953	1.00	5.50
ATOM	367	CB	GLU A	66	16.894	23.810	3.685	1.00	6.69
ATOM	368	CG	GLU A	66	17.515	24.418	2.501	1.00	13.05
ATOM	369	CD	GLU A	66	17.003	23.830	1.239	1.00	14.87
ATOM	370	OE1	GLU A	66	16.957	22.580	1.173	1.00	21.13
ATOM	371	OE2	GLU A	66	16.662	24.612	0.317	1.00	20.98
ATOM	372	C	GLU A	66	17.369	25.630	5.396	1.00	7.85
ATOM	373	O	GLU A	66	16.276	25.972	5.831	1.00	9.32
ATOM	374	N	VAL A	67	18.425	26.450	5.345	1.00	2.00
ATOM	375	CA	VAL A	67	18.338	27.862	5.760	1.00	2.00
ATOM	376	CB	VAL A	67	19.092	28.115	7.090	1.00	4.04
ATOM	377	CG1	VAL A	67	18.431	27.338	8.255	1.00	4.42
ATOM	378	CG2	VAL A	67	20.566	27.742	6.938	1.00	2.00
ATOM	379	C	VAL A	67	18.904	28.826	4.689	1.00	2.30
ATOM	380	O	VAL A	67	18.836	30.057	4.779	1.00	2.00
ATOM	381	N	GLY A	68	19.450	28.248	3.635	1.00	2.00
ATOM	382	CA	GLY A	68	20.025	29.075	2.597	1.00	2.48
ATOM	383	C	GLY A	68	20.409	28.329	1.331	1.00	5.80
ATOM	384	O	GLY A	68	20.007	27.176	1.121	1.00	5.04
ATOM	385	N	ARG A	69	21.206	28.992	0.497	1.00	4.71
ATOM	386	CA	ARG A	69	21.633	28.441	-0.800	1.00	2.93
ATOM	387	CB	ARG A	69	20.607	28.868	-1.840	1.00	5.96
ATOM	388	CG	ARG A	69	20.876	28.429	-3.240	1.00	2.76
ATOM	389	CD	ARG A	69	20.782	26.944	-3.325	1.00	12.84
ATOM	390	NE	ARG A	69	19.420	26.446	-3.154	1.00	20.69
ATOM	391	CZ	ARG A	69	18.414	26.726	-3.981	1.00	26.00
ATOM	392	NH1	ARG A	69	17.222	26.189	-3.755	1.00	31.06
ATOM	393	NH2	ARG A	69	18.575	27.566	-5.005	1.00	19.94
ATOM	394	C	ARG A	69	23.039	28.947	-1.181	1.00	7.65
ATOM	395	O	ARG A	69	23.357	30.142	-1.074	1.00	10.32
ATOM	396	N	VAL A	70	23.890	28.003	-1.572	1.00	3.09
ATOM	397	CA	VAL A	70	25.255	28.293	-2.032	1.00	4.52
ATOM	398	CB	VAL A	70	26.003	26.973	-2.298	1.00	7.64
ATOM	399	CG1	VAL A	70	27.218	27.213	-3.172	1.00	4.40
ATOM	400	CG2	VAL A	70	26.394	26.316	-0.990	1.00	2.00
ATOM	401	C	VAL A	70	25.131	29.074	-3.370	1.00	5.74
ATOM	402	O	VAL A	70	24.599	28.572	-4.371	1.00	8.25
ATOM	403	N	LEU A	71	25.586	30.323	-3.365	1.00	3.92
ATOM	404	CA	LEU A	71	25.536	31.164	-4.598	1.00	4.53
ATOM	405	CB	LEU A	71	25.626	32.632	-4.222	1.00	2.00
ATOM	406	CG	LEU A	71	24.540	33.220	-3.364	1.00	2.00
ATOM	407	CD1	LEU A	71	24.895	34.632	-3.013	1.00	2.00
ATOM	408	CD2	LEU A	71	23.235	33.127	-4.095	1.00	3.70
ATOM	409	C	LEU A	71	26.640	30.834	-5.664	1.00	9.13
ATOM	410	O	LEU A	71	26.368	30.776	-6.879	1.00	9.84
ATOM	411	N	ALA A	72	27.886	30.666	-5.188	1.00	6.69
ATOM	412	CA	ALA A	72	29.052	30.374	-6.057	1.00	4.02
ATOM	413	CB	ALA A	72	29.666	31.650	-6.519	1.00	3.51
ATOM	414	C	ALA A	72	30.126	29.535	-5.401	1.00	4.92
ATOM	415	O	ALA A	72	30.435	29.665	-4.233	1.00	11.03

Fig. 4I

ATOM	416	N	VAL	A	73	30.707	28.653	-6.201	1.00	10.43
ATOM	417	CA	VAL	A	73	31.820	27.777	-5.771	1.00	6.81
ATOM	418	CB	VAL	A	73	31.430	26.308	-5.804	1.00	2.00
ATOM	419	CG1	VAL	A	73	32.555	25.455	-5.236	1.00	2.00
ATOM	420	CG2	VAL	A	73	30.189	26.099	-5.002	1.00	5.59
ATOM	421	C	VAL	A	73	32.883	28.024	-6.848	1.00	8.19
ATOM	422	O	VAL	A	73	32.647	27.820	-8.022	1.00	11.49
ATOM	423	N	VAL	A	74	34.024	28.575	-6.461	1.00	9.12
ATOM	424	CA	VAL	A	74	35.096	28.841	-7.432	1.00	12.05
ATOM	425	CB	VAL	A	74	35.448	30.326	-7.505	1.00	14.05
ATOM	426	CG1	VAL	A	74	36.561	30.545	-8.508	1.00	24.53
ATOM	427	CG2	VAL	A	74	34.247	31.120	-7.923	1.00	18.08
ATOM	428	C	VAL	A	74	36.347	28.070	-7.028	1.00	5.85
ATOM	429	O	VAL	A	74	36.768	28.042	-5.872	1.00	20.53
ATOM	430	N	ASN	A	75	36.950	27.410	-8.005	1.00	18.46
ATOM	431	CA	ASN	A	75	38.184	26.631	-7.742	1.00	15.45
ATOM	432	CB	ASN	A	75	38.390	25.617	-8.861	1.00	13.02
ATOM	433	CG	ASN	A	75	39.521	24.674	-8.588	1.00	17.82
ATOM	434	OD1	ASN	A	75	39.685	23.691	-9.285	1.00	23.74
ATOM	435	ND2	ASN	A	75	40.301	24.941	-7.556	1.00	25.51
ATOM	436	C	ASN	A	75	39.368	27.612	-7.622	1.00	15.03
ATOM	437	O	ASN	A	75	39.864	28.196	-8.580	1.00	21.05
ATOM	438	N	ASP	A	76	39.763	27.857	-6.389	1.00	11.85
ATOM	439	CA	ASP	A	76	40.876	28.758	-6.129	1.00	7.24
ATOM	440	CB	ASP	A	76	40.668	29.441	-4.799	1.00	6.29
ATOM	441	CG	ASP	A	76	41.737	30.428	-4.504	1.00	5.01
ATOM	442	OD1	ASP	A	76	42.770	30.070	-3.923	1.00	13.20
ATOM	443	OD2	ASP	A	76	41.582	31.575	-4.905	1.00	6.55
ATOM	444	C	ASP	A	76	42.117	27.891	-6.081	1.00	11.98
ATOM	445	O	ASP	A	76	42.051	26.707	-5.724	1.00	14.65
ATOM	446	N	PRO	A	77	43.286	28.467	-6.428	1.00	12.34
ATOM	447	CD	PRO	A	77	43.528	29.807	-6.995	1.00	11.81
ATOM	448	CA	PRO	A	77	44.536	27.705	-6.402	1.00	12.16
ATOM	449	CB	PRO	A	77	45.587	28.793	-6.606	1.00	7.70
ATOM	450	CG	PRO	A	77	44.942	29.716	-7.505	1.00	4.35
ATOM	451	C	PRO	A	77	44.754	26.967	-5.057	1.00	8.68
ATOM	452	O	PRO	A	77	45.498	26.013	-4.963	1.00	13.91
ATOM	453	N	ARG	A	78	44.080	27.430	-4.019	1.00	6.30
ATOM	454	CA	ARG	A	78	44.198	26.819	-2.693	1.00	6.81
ATOM	455	CB	ARG	A	78	44.216	27.920	-1.654	1.00	10.10
ATOM	456	CG	ARG	A	78	45.331	28.956	-1.816	1.00	17.49
ATOM	457	CD	ARG	A	78	45.291	29.994	-0.688	1.00	18.69
ATOM	458	NE	ARG	A	78	45.447	29.361	0.633	1.00	31.64
ATOM	459	CZ	ARG	A	78	44.803	29.705	1.754	1.00	33.18
ATOM	460	NH1	ARG	A	78	45.054	29.035	2.869	1.00	29.53
ATOM	461	NH2	ARG	A	78	43.909	30.696	1.771	1.00	33.74
ATOM	462	C	ARG	A	78	43.096	25.762	-2.361	1.00	7.54
ATOM	463	O	ARG	A	78	43.277	24.854	-1.558	1.00	6.14
ATOM	464	N	GLY	A	79	41.959	25.860	-3.023	1.00	5.69
ATOM	465	CA	GLY	A	79	40.890	24.922	-2.748	1.00	4.76
ATOM	466	C	GLY	A	79	39.569	25.503	-3.201	1.00	2.72
ATOM	467	O	GLY	A	79	39.493	26.685	-3.550	1.00	5.32

Fig. 4J

ATOM	468	N	PRO	A	80	38.509	24.705	-3.203	1.00	2.00
ATOM	469	CD	PRO	A	80	38.451	23.305	-2.747	1.00	9.44
ATOM	470	CA	PRO	A	80	37.195	25.181	-3.626	1.00	2.00
ATOM	471	CB	PRO	A	80	36.351	23.910	-3.643	1.00	4.12
ATOM	472	CG	PRO	A	80	36.937	23.081	-2.554	1.00	7.73
ATOM	473	C	PRO	A	80	36.671	26.145	-2.591	1.00	5.31
ATOM	474	O	PRO	A	80	36.447	25.789	-1.433	1.00	4.34
ATOM	475	N	PHE	A	81	36.478	27.382	-3.028	1.00	2.00
ATOM	476	CA	PHE	A	81	35.980	28.451	-2.177	1.00	2.00
ATOM	477	CB	PHE	A	81	36.820	29.678	-2.460	1.00	2.00
ATOM	478	CG	PHE	A	81	36.469	30.865	-1.616	1.00	3.57
ATOM	479	CD1	PHE	A	81	37.002	31.014	-0.344	1.00	2.00
ATOM	480	CD2	PHE	A	81	35.626	31.852	-2.103	1.00	5.30
ATOM	481	CE1	PHE	A	81	36.704	32.113	0.410	1.00	2.00
ATOM	482	CE2	PHE	A	81	35.325	32.967	-1.331	1.00	3.68
ATOM	483	CZ	PHE	A	81	35.865	33.091	-0.081	1.00	2.00
ATOM	484	C	PHE	A	81	34.502	28.681	-2.531	1.00	7.75
ATOM	485	O	PHE	A	81	34.112	28.576	-3.685	1.00	15.16
ATOM	486	N	PHE	A	82	33.664	29.007	-1.554	1.00	6.33
ATOM	487	CA	PHE	A	82	32.242	29.232	-1.873	1.00	4.82
ATOM	488	CB	PHE	A	82	31.422	27.997	-1.496	1.00	6.81
ATOM	489	CG	PHE	A	82	30.867	28.042	-0.102	1.00	4.39
ATOM	490	CD1	PHE	A	82	31.695	27.858	1.007	1.00	8.36
ATOM	491	CD2	PHE	A	82	29.521	28.326	0.113	1.00	6.71
ATOM	492	CE1	PHE	A	82	31.184	27.967	2.313	1.00	2.00
ATOM	493	CE2	PHE	A	82	29.003	28.437	1.416	1.00	2.00
ATOM	494	CZ	PHE	A	82	29.826	28.261	2.506	1.00	2.00
ATOM	495	C	PHE	A	82	31.658	30.467	-1.186	1.00	6.36
ATOM	496	O	PHE	A	82	32.196	31.009	-0.222	1.00	10.33
ATOM	497	N	VAL	A	83	30.528	30.916	-1.711	1.00	4.44
ATOM	498	CA	VAL	A	83	29.814	32.038	-1.130	1.00	2.00
ATOM	499	CB	VAL	A	83	30.015	33.276	-1.924	1.00	3.99
ATOM	500	CG1	VAL	A	83	29.023	34.322	-1.503	1.00	2.78
ATOM	501	CG2	VAL	A	83	31.425	33.791	-1.678	1.00	13.68
ATOM	502	C	VAL	A	83	28.341	31.663	-1.106	1.00	3.33
ATOM	503	O	VAL	A	83	27.759	31.273	-2.111	1.00	2.00
ATOM	504	N	GLY	A	84	27.756	31.739	0.089	1.00	5.01
ATOM	505	CA	GLY	A	84	26.361	31.403	0.276	1.00	2.00
ATOM	506	C	GLY	A	84	25.521	32.507	0.877	1.00	3.07
ATOM	507	O	GLY	A	84	26.021	33.514	1.368	1.00	3.16
ATOM	508	N	LEU	A	85	24.214	32.300	0.813	1.00	5.57
ATOM	509	CA	LEU	A	85	23.225	33.244	1.345	1.00	6.55
ATOM	510	CB	LEU	A	85	22.446	33.914	0.204	1.00	9.10
ATOM	511	CG	LEU	A	85	21.273	34.832	0.602	1.00	13.82
ATOM	512	CD1	LEU	A	85	21.742	36.213	1.049	1.00	10.07
ATOM	513	CD2	LEU	A	85	20.340	34.954	-0.574	1.00	15.04
ATOM	514	C	LEU	A	85	22.261	32.507	2.284	1.00	4.79
ATOM	515	O	LEU	A	85	21.641	31.512	1.946	1.00	3.64
ATOM	516	N	ILE	A	86	22.079	33.084	3.454	1.00	5.27
ATOM	517	CA	ILE	A	86	21.205	32.530	4.479	1.00	3.56
ATOM	518	CB	ILE	A	86	22.028	32.326	5.749	1.00	2.77
ATOM	519	CG2	ILE	A	86	21.167	31.976	6.944	1.00	2.00

Fig. 4K

ATOM	520	CG1	ILE	A	86	23.096	31.285	5.462	1.00	2.00
ATOM	521	CD1	ILE	A	86	24.264	31.383	6.391	1.00	4.00
ATOM	522	C	ILE	A	86	20.123	33.590	4.702	1.00	4.40
ATOM	523	O	ILE	A	86	20.391	34.729	5.083	1.00	10.66
ATOM	524	N	ALA	A	87	18.895	33.243	4.364	1.00	2.00
ATOM	525	CA	ALA	A	87	17.769	34.182	4.546	1.00	2.63
ATOM	526	CB	ALA	A	87	17.195	34.573	3.209	1.00	2.00
ATOM	527	C	ALA	A	87	16.769	33.359	5.373	1.00	4.47
ATOM	528	O	ALA	A	87	15.911	32.647	4.852	1.00	8.98
ATOM	529	N	CYS	A	88	16.915	33.457	6.690	1.00	2.00
ATOM	530	CA	CYS	A	88	16.103	32.696	7.618	1.00	2.00
ATOM	531	CB	CYS	A	88	16.808	31.403	7.904	1.00	2.00
ATOM	532	SG	CYS	A	88	15.896	30.256	8.869	1.00	8.13
ATOM	533	C	CYS	A	88	15.933	33.490	8.887	1.00	8.16
ATOM	534	O	CYS	A	88	16.888	33.696	9.630	1.00	15.01
ATOM	535	N	VAL	A	89	14.686	33.892	9.151	1.00	9.38
ATOM	536	CA	VAL	A	89	14.304	34.687	10.324	1.00	5.40
ATOM	537	CB	VAL	A	89	13.011	35.449	10.038	1.00	10.95
ATOM	538	CG1	VAL	A	89	11.818	34.490	9.928	1.00	17.11
ATOM	539	CG2	VAL	A	89	12.776	36.474	11.101	1.00	18.15
ATOM	540	C	VAL	A	89	14.146	33.847	11.593	1.00	6.11
ATOM	541	O	VAL	A	89	14.405	34.285	12.704	1.00	7.14
ATOM	542	N	GLN	A	90	13.743	32.596	11.409	1.00	8.62
ATOM	543	CA	GLN	A	90	13.560	31.676	12.558	1.00	10.52
ATOM	544	CB	GLN	A	90	12.874	30.382	12.105	1.00	9.44
ATOM	545	CG	GLN	A	90	11.509	30.622	11.532	1.00	10.44
ATOM	546	CD	GLN	A	90	10.788	29.349	11.176	1.00	9.31
ATOM	547	OE1	GLN	A	90	11.395	28.352	10.832	1.00	11.38
ATOM	548	NE2	GLN	A	90	9.483	29.381	11.256	1.00	7.37
ATOM	549	C	GLN	A	90	14.912	31.386	13.225	1.00	10.11
ATOM	550	O	GLN	A	90	15.032	31.318	14.451	1.00	13.62
ATOM	551	N	LEU	A	91	15.912	31.162	12.378	1.00	8.00
ATOM	552	CA	LEU	A	91	17.302	30.911	12.807	1.00	8.35
ATOM	553	CB	LEU	A	91	18.165	30.723	11.572	1.00	11.36
ATOM	554	CG	LEU	A	91	19.674	30.578	11.747	1.00	11.77
ATOM	555	CD1	LEU	A	91	19.995	29.420	12.673	1.00	12.66
ATOM	556	CD2	LEU	A	91	20.305	30.390	10.389	1.00	7.29
ATOM	557	C	LEU	A	91	17.774	32.130	13.638	1.00	10.15
ATOM	558	O	LEU	A	91	18.449	31.984	14.644	1.00	6.95
ATOM	559	N	GLU	A	92	17.391	33.327	13.180	1.00	9.63
ATOM	560	CA	GLU	A	92	17.691	34.611	13.874	1.00	12.76
ATOM	561	CB	GLU	A	92	17.091	35.810	13.140	1.00	12.46
ATOM	562	CG	GLU	A	92	17.655	36.034	11.770	1.00	21.61
ATOM	563	CD	GLU	A	92	17.159	37.312	11.128	1.00	22.26
ATOM	564	OE1	GLU	A	92	17.145	37.365	9.871	1.00	14.51
ATOM	565	OE2	GLU	A	92	16.811	38.259	11.880	1.00	22.36
ATOM	566	C	GLU	A	92	17.113	34.600	15.273	1.00	14.56
ATOM	567	O	GLU	A	92	17.820	34.756	16.257	1.00	18.51
ATOM	568	N	ARG	A	93	15.789	34.447	15.340	1.00	16.39
ATOM	569	CA	ARG	A	93	15.034	34.420	16.618	1.00	11.28
ATOM	570	CB	ARG	A	93	13.555	34.263	16.325	1.00	19.47
ATOM	571	CG	ARG	A	93	13.043	35.267	15.317	1.00	33.53

Fig. 4L

ATOM	572	CD	ARG	A	93	13.303	36.728	15.717	1.00	45.19
ATOM	573	NE	ARG	A	93	12.803	37.635	14.671	1.00	57.43
ATOM	574	CZ	ARG	A	93	12.734	38.965	14.766	1.00	58.50
ATOM	575	NH1	ARG	A	93	12.254	39.681	13.744	1.00	55.89
ATOM	576	NH2	ARG	A	93	13.134	39.583	15.874	1.00	63.25
ATOM	577	C	ARG	A	93	15.502	33.355	17.594	1.00	7.89
ATOM	578	O	ARG	A	93	15.806	33.641	18.738	1.00	12.57
ATOM	579	N	VAL	A	94	15.514	32.104	17.147	1.00	9.52
ATOM	580	CA	VAL	A	94	15.980	30.944	17.982	1.00	9.28
ATOM	581	CB	VAL	A	94	16.129	29.677	17.106	1.00	8.75
ATOM	582	CG1	VAL	A	94	16.944	28.652	17.794	1.00	3.33
ATOM	583	CG2	VAL	A	94	14.779	29.132	16.743	1.00	2.00
ATOM	584	C	VAL	A	94	17.341	31.254	18.682	1.00	11.69
ATOM	585	O	VAL	A	94	17.529	30.958	19.849	1.00	16.80
ATOM	586	N	LEU	A	95	18.275	31.852	17.930	1.00	13.58
ATOM	587	CA	LEU	A	95	19.654	32.266	18.403	1.00	9.12
ATOM	588	CB	LEU	A	95	20.525	32.603	17.186	1.00	6.38
ATOM	589	CG	LEU	A	95	21.859	31.898	16.895	1.00	10.10
ATOM	590	CD1	LEU	A	95	21.871	30.426	17.327	1.00	3.73
ATOM	591	CD2	LEU	A	95	22.163	32.031	15.409	1.00	2.00
ATOM	592	C	LEU	A	95	19.563	33.499	19.352	1.00	13.12
ATOM	593	O	LEU	A	95	20.104	33.521	20.446	1.00	13.37
ATOM	594	N	GLU	A	96	18.887	34.539	18.873	1.00	13.34
ATOM	595	CA	GLU	A	96	18.659	35.804	19.629	1.00	17.07
ATOM	596	CB	GLU	A	96	17.734	36.757	18.853	1.00	19.22
ATOM	597	CG	GLU	A	96	18.408	37.707	17.868	1.00	32.52
ATOM	598	CD	GLU	A	96	17.406	38.554	17.059	1.00	38.30
ATOM	599	OE1	GLU	A	96	17.825	39.156	16.026	1.00	43.55
ATOM	600	OE2	GLU	A	96	16.205	38.612	17.448	1.00	37.03
ATOM	601	C	GLU	A	96	18.035	35.572	21.013	1.00	19.12
ATOM	602	O	GLU	A	96	18.311	36.270	21.987	1.00	22.88
ATOM	603	N	THR	A	97	17.101	34.635	21.069	1.00	16.70
ATOM	604	CA	THR	A	97	16.412	34.372	22.330	1.00	13.97
ATOM	605	CB	THR	A	97	14.913	33.848	22.102	1.00	16.11
ATOM	606	OG1	THR	A	97	14.907	32.571	21.446	1.00	17.85
ATOM	607	CG2	THR	A	97	14.131	34.796	21.229	1.00	8.17
ATOM	608	C	THR	A	97	17.220	33.430	23.234	1.00	14.30
ATOM	609	O	THR	A	97	17.150	33.500	24.456	1.00	21.32
ATOM	610	N	ALA	A	98	17.985	32.528	22.626	1.00	13.54
ATOM	611	CA	ALA	A	98	18.795	31.570	23.418	1.00	11.87
ATOM	612	CB	ALA	A	98	19.441	30.531	22.509	1.00	13.72
ATOM	613	C	ALA	A	98	19.864	32.364	24.134	1.00	7.51
ATOM	614	O	ALA	A	98	20.184	32.156	25.275	1.00	14.36
ATOM	615	N	ALA	A	99	20.422	33.316	23.419	1.00	11.45
ATOM	616	CA	ALA	A	99	21.467	34.153	23.964	1.00	15.58
ATOM	617	CB	ALA	A	99	22.039	35.055	22.873	1.00	6.98
ATOM	618	C	ALA	A	99	20.887	35.000	25.077	1.00	23.42
ATOM	619	O	ALA	A	99	20.260	36.027	24.851	1.00	27.39
ATOM	620	N	SER	A	100	21.074	34.551	26.308	1.00	32.15
ATOM	621	CA	SER	A	100	20.618	35.352	27.493	1.00	39.64
ATOM	622	CB	SER	A	100	20.268	34.422	28.668	1.00	43.91
ATOM	623	OG	SER	A	100	19.189	33.539	28.344	1.00	42.68

Fig. 4M

ATOM	624	C	SER A 100	21.921	36.163	27.718	1.00	38.85
ATOM	625	O	SER A 100	22.580	36.190	28.753	1.00	34.35
ATOM	626	N	ALA A 101	22.272	36.809	26.619	1.00	42.20
ATOM	627	CA	ALA A 101	23.483	37.575	26.483	1.00	48.71
ATOM	628	CB	ALA A 101	23.616	38.111	25.044	1.00	48.97
ATOM	629	C	ALA A 101	23.751	38.676	27.480	1.00	52.91
ATOM	630	O	ALA A 101	22.903	39.483	27.879	1.00	51.94
ATOM	631	N	ALA A 102	25.000	38.637	27.910	1.00	56.37
ATOM	632	CA	ALA A 102	25.550	39.612	28.800	1.00	59.62
ATOM	633	CB	ALA A 102	26.570	38.960	29.679	1.00	61.10
ATOM	634	C	ALA A 102	26.223	40.477	27.723	1.00	63.57
ATOM	635	O	ALA A 102	25.807	41.600	27.410	1.00	66.92
ATOM	636	N	ALA A 103	27.198	39.855	27.060	1.00	64.90
ATOM	637	CA	ALA A 103	27.969	40.496	25.958	1.00	64.92
ATOM	638	CB	ALA A 103	29.159	41.292	26.514	1.00	63.32
ATOM	639	C	ALA A 103	28.456	39.397	24.981	1.00	64.15
ATOM	640	O	ALA A 103	28.807	39.751	23.838	1.00	64.98
ATOM	641	OT	ALA A 103	28.431	38.200	25.360	1.00	64.17
ATOM	642	CB	LEU A 111	26.747	44.455	20.372	1.00	56.29
ATOM	643	CG	LEU A 111	27.624	44.132	19.156	1.00	54.59
ATOM	644	CD1	LEU A 111	28.799	45.121	18.988	1.00	51.56
ATOM	645	CD2	LEU A 111	28.112	42.683	19.301	1.00	52.46
ATOM	646	C	LEU A 111	25.766	46.776	19.890	1.00	58.98
ATOM	647	O	LEU A 111	25.724	48.011	20.026	1.00	60.58
ATOM	648	N	LEU A 111	25.687	45.879	22.111	1.00	60.93
ATOM	649	CA	LEU A 111	26.541	45.892	20.888	1.00	59.20
ATOM	650	N	SER A 112	25.096	46.141	18.932	1.00	55.16
ATOM	651	CA	SER A 112	24.314	46.915	17.974	1.00	51.29
ATOM	652	CB	SER A 112	25.164	47.301	16.768	1.00	53.00
ATOM	653	OG	SER A 112	26.127	48.277	17.146	1.00	59.40
ATOM	654	C	SER A 112	22.994	46.330	17.540	1.00	48.24
ATOM	655	O	SER A 112	21.948	46.720	18.039	1.00	52.52
ATOM	656	N	ARG A 113	23.032	45.323	16.678	1.00	43.61
ATOM	657	CA	ARG A 113	21.765	44.782	16.147	1.00	40.68
ATOM	658	CB	ARG A 113	21.251	45.872	15.247	1.00	46.02
ATOM	659	CG	ARG A 113	22.407	46.709	14.618	1.00	53.20
ATOM	660	CD	ARG A 113	22.013	47.317	13.295	1.00	68.22
ATOM	661	NE	ARG A 113	20.629	47.807	13.317	1.00	78.52
ATOM	662	CZ	ARG A 113	19.562	47.071	12.992	1.00	82.20
ATOM	663	NH1	ARG A 113	18.342	47.604	13.052	1.00	85.11
ATOM	664	NH2	ARG A 113	19.707	45.800	12.627	1.00	83.47
ATOM	665	C	ARG A 113	21.936	43.443	15.397	1.00	39.97
ATOM	666	O	ARG A 113	22.039	42.363	15.964	1.00	39.56
ATOM	667	N	GLU A 114	21.934	43.524	14.075	1.00	37.09
ATOM	668	CA	GLU A 114	22.175	42.332	13.265	1.00	34.54
ATOM	669	CB	GLU A 114	21.901	42.632	11.786	1.00	38.06
ATOM	670	CG	GLU A 114	22.674	43.797	11.194	1.00	44.41
ATOM	671	CD	GLU A 114	21.784	44.832	10.494	1.00	46.14
ATOM	672	OE1	GLU A 114	20.608	44.533	10.181	1.00	43.86
ATOM	673	OE2	GLU A 114	22.270	45.963	10.261	1.00	50.76
ATOM	674	C	GLU A 114	23.648	41.888	13.520	1.00	31.23
ATOM	675	O	GLU A 114	24.063	40.781	13.208	1.00	32.58

Fig. 4N

ATOM	676	N	GLU A 115	24.433	42.784	14.112	1.00	24.68
ATOM	677	CA	GLU A 115	25.838	42.476	14.465	1.00	21.27
ATOM	678	CB	GLU A 115	26.582	43.757	14.818	1.00	23.85
ATOM	679	CG	GLU A 115	27.051	44.517	13.572	1.00	34.75
ATOM	680	CD	GLU A 115	27.060	46.036	13.728	1.00	42.96
ATOM	681	OE1	GLU A 115	27.517	46.540	14.786	1.00	45.07
ATOM	682	OE2	GLU A 115	26.622	46.724	12.770	1.00	45.48
ATOM	683	C	GLU A 115	25.815	41.468	15.617	1.00	18.01
ATOM	684	O	GLU A 115	26.614	40.547	15.712	1.00	16.83
ATOM	685	N	ARG A 116	24.819	41.629	16.476	1.00	17.08
ATOM	686	CA	ARG A 116	24.616	40.713	17.602	1.00	13.12
ATOM	687	CB	ARG A 116	23.423	41.200	18.420	1.00	23.37
ATOM	688	CG	ARG A 116	23.715	41.525	19.891	1.00	40.43
ATOM	689	CD	ARG A 116	23.791	40.244	20.790	1.00	50.89
ATOM	690	NE	ARG A 116	24.307	40.566	22.119	1.00	51.56
ATOM	691	CZ	ARG A 116	25.503	40.230	22.595	1.00	50.96
ATOM	692	NH1	ARG A 116	26.357	39.495	21.894	1.00	50.65
ATOM	693	NH2	ARG A 116	25.930	40.837	23.684	1.00	48.08
ATOM	694	C	ARG A 116	24.330	39.344	16.948	1.00	9.40
ATOM	695	O	ARG A 116	24.761	38.293	17.376	1.00	10.43
ATOM	696	N	LEU A 117	23.592	39.388	15.853	1.00	8.24
ATOM	697	CA	LEU A 117	23.256	38.181	15.130	1.00	5.12
ATOM	698	CB	LEU A 117	22.198	38.486	14.082	1.00	11.72
ATOM	699	CG	LEU A 117	21.910	37.396	13.046	1.00	14.16
ATOM	700	CD1	LEU A 117	21.610	36.054	13.696	1.00	11.49
ATOM	701	CD2	LEU A 117	20.762	37.846	12.186	1.00	17.08
ATOM	702	C	LEU A 117	24.503	37.611	14.495	1.00	6.75
ATOM	703	O	LEU A 117	24.755	36.403	14.538	1.00	10.82
ATOM	704	N	LEU A 118	25.308	38.489	13.895	1.00	10.20
ATOM	705	CA	LEU A 118	26.584	38.053	13.226	1.00	8.45
ATOM	706	CB	LEU A 118	27.275	39.227	12.548	1.00	7.18
ATOM	707	CG	LEU A 118	27.047	39.365	11.050	1.00	2.10
ATOM	708	CD1	LEU A 118	26.269	38.175	10.493	1.00	2.00
ATOM	709	CD2	LEU A 118	26.379	40.655	10.807	1.00	2.00
ATOM	710	C	LEU A 118	27.517	37.406	14.234	1.00	7.43
ATOM	711	O	LEU A 118	28.079	36.328	14.013	1.00	4.46
ATOM	712	N	TYR A 119	27.601	38.060	15.388	1.00	5.07
ATOM	713	CA	TYR A 119	28.443	37.599	16.496	1.00	11.79
ATOM	714	CB	TYR A 119	28.461	38.650	17.626	1.00	14.97
ATOM	715	CG	TYR A 119	29.115	38.152	18.895	1.00	20.96
ATOM	716	CD1	TYR A 119	28.408	37.339	19.794	1.00	26.44
ATOM	717	CE1	TYR A 119	28.995	36.828	20.938	1.00	30.15
ATOM	718	CD2	TYR A 119	30.441	38.452	19.184	1.00	25.49
ATOM	719	CE2	TYR A 119	31.048	37.949	20.338	1.00	31.21
ATOM	720	CZ	TYR A 119	30.313	37.133	21.204	1.00	35.37
ATOM	721	OH	TYR A 119	30.895	36.586	22.322	1.00	43.14
ATOM	722	C	TYR A 119	27.960	36.227	16.991	1.00	10.78
ATOM	723	O	TYR A 119	28.738	35.296	17.238	1.00	17.49
ATOM	724	N	LEU A 120	26.645	36.102	17.119	1.00	10.50
ATOM	725	CA	LEU A 120	26.017	34.833	17.584	1.00	7.62
ATOM	726	CB	LEU A 120	24.540	35.090	17.881	1.00	7.13
ATOM	727	CG	LEU A 120	23.932	34.993	19.283	1.00	9.79

Fig. 40

ATOM	728	CD1	LEU	A	120	24.953	35.123	20.382	1.00	10.87
ATOM	729	CD2	LEU	A	120	22.866	36.058	19.416	1.00	6.08
ATOM	730	C	LEU	A	120	26.197	33.666	16.592	1.00	5.17
ATOM	731	O	LEU	A	120	26.630	32.578	16.967	1.00	4.21
ATOM	732	N	ILE	A	121	25.911	33.890	15.306	1.00	6.28
ATOM	733	CA	ILE	A	121	26.046	32.758	14.333	1.00	4.47
ATOM	734	CB	ILE	A	121	25.227	32.973	13.005	1.00	4.54
ATOM	735	CG2	ILE	A	121	25.844	34.013	12.150	1.00	2.00
ATOM	736	CG1	ILE	A	121	25.179	31.673	12.203	1.00	5.33
ATOM	737	CD1	ILE	A	121	24.105	31.640	11.167	1.00	2.00
ATOM	738	C	ILE	A	121	27.508	32.340	14.073	1.00	3.60
ATOM	739	O	ILE	A	121	27.831	31.150	14.057	1.00	5.52
ATOM	740	N	THR	A	122	28.401	33.329	13.965	1.00	2.00
ATOM	741	CA	THR	A	122	29.845	33.076	13.723	1.00	2.00
ATOM	742	CB	THR	A	122	30.641	34.347	13.741	1.00	2.00
ATOM	743	OG1	THR	A	122	30.071	35.275	12.822	1.00	7.60
ATOM	744	CG2	THR	A	122	32.064	34.055	13.321	1.00	5.83
ATOM	745	C	THR	A	122	30.520	32.170	14.742	1.00	2.73
ATOM	746	O	THR	A	122	31.240	31.224	14.415	1.00	6.41
ATOM	747	N	ASN	A	123	30.352	32.521	16.009	1.00	5.60
ATOM	748	CA	ASN	A	123	30.966	31.748	17.094	1.00	2.00
ATOM	749	CB	ASN	A	123	31.109	32.621	18.320	1.00	5.03
ATOM	750	CG	ASN	A	123	31.976	33.843	18.062	1.00	7.80
ATOM	751	OD1	ASN	A	123	31.485	34.951	17.920	1.00	5.81
ATOM	752	ND2	ASN	A	123	33.259	33.631	17.952	1.00	4.02
ATOM	753	C	ASN	A	123	30.266	30.443	17.415	1.00	4.01
ATOM	754	O	ASN	A	123	30.865	29.534	17.965	1.00	6.29
ATOM	755	N	TYR	A	124	28.982	30.342	17.089	1.00	2.98
ATOM	756	CA	TYR	A	124	28.238	29.070	17.342	1.00	3.33
ATOM	757	CB	TYR	A	124	26.721	29.293	17.531	1.00	2.24
ATOM	758	CG	TYR	A	124	26.043	28.123	18.215	1.00	3.71
ATOM	759	CD1	TYR	A	124	26.249	27.882	19.575	1.00	6.66
ATOM	760	CE1	TYR	A	124	25.678	26.797	20.214	1.00	3.17
ATOM	761	CD2	TYR	A	124	25.232	27.230	17.510	1.00	4.38
ATOM	762	CE2	TYR	A	124	24.651	26.140	18.148	1.00	2.75
ATOM	763	CZ	TYR	A	124	24.880	25.930	19.503	1.00	4.23
ATOM	764	OH	TYR	A	124	24.331	24.850	20.179	1.00	4.84
ATOM	765	C	TYR	A	124	28.468	28.114	16.166	1.00	2.60
ATOM	766	O	TYR	A	124	28.690	26.933	16.322	1.00	5.11
ATOM	767	N	LEU	A	125	28.368	28.656	14.964	1.00	4.89
ATOM	768	CA	LEU	A	125	28.552	27.858	13.757	1.00	9.24
ATOM	769	CB	LEU	A	125	27.240	27.849	12.972	1.00	6.85
ATOM	770	CG	LEU	A	125	26.063	27.110	13.626	1.00	2.89
ATOM	771	CD1	LEU	A	125	24.860	27.277	12.737	1.00	2.00
ATOM	772	CD2	LEU	A	125	26.361	25.631	13.854	1.00	2.00
ATOM	773	C	LEU	A	125	29.734	28.380	12.913	1.00	9.42
ATOM	774	O	LEU	A	125	29.572	28.868	11.804	1.00	8.71
ATOM	775	N	PRO	A	126	30.965	28.210	13.430	1.00	11.38
ATOM	776	CD	PRO	A	126	31.309	27.672	14.764	1.00	4.65
ATOM	777	CA	PRO	A	126	32.164	28.675	12.722	1.00	7.79
ATOM	778	CB	PRO	A	126	33.187	28.769	13.849	1.00	5.75
ATOM	779	CG	PRO	A	126	32.801	27.662	14.764	1.00	2.00

Fig. 4P

ATOM	780	C	PRO A 126	32.704	27.870	11.495	1.00	7.74
ATOM	781	O	PRO A 126	33.521	28.396	10.727	1.00	9.84
ATOM	782	N	SER A 127	32.204	26.649	11.275	1.00	2.00
ATOM	783	CA	SER A 127	32.669	25.783	10.146	1.00	2.00
ATOM	784	CB	SER A 127	33.270	24.508	10.731	1.00	2.00
ATOM	785	OG	SER A 127	34.258	24.800	11.690	1.00	2.49
ATOM	786	C	SER A 127	31.674	25.377	9.036	1.00	2.00
ATOM	787	O	SER A 127	30.463	25.486	9.164	1.00	2.00
ATOM	788	N	VAL A 128	32.222	24.903	7.920	1.00	2.00
ATOM	789	CA	VAL A 128	31.380	24.368	6.809	1.00	4.25
ATOM	790	CB	VAL A 128	31.641	24.922	5.406	1.00	5.15
ATOM	791	CG1	VAL A 128	30.631	25.964	5.077	1.00	14.62
ATOM	792	CG2	VAL A 128	33.039	25.411	5.261	1.00	3.69
ATOM	793	C	VAL A 128	31.775	22.937	6.678	1.00	5.33
ATOM	794	O	VAL A 128	32.845	22.503	7.066	1.00	8.22
ATOM	795	P1	SEI A 129	31.695	17.762	7.461	1.00	8.79
ATOM	796	O3	SEI A 129	31.372	17.687	9.055	1.00	11.54
ATOM	797	O4	SEI A 129	31.616	16.285	6.832	1.00	7.78
ATOM	798	O5	SEI A 129	30.630	18.671	6.720	1.00	9.57
ATOM	799	C5	SEI A 129	30.226	17.113	9.752	1.00	10.71
ATOM	800	C6	SEI A 129	30.679	16.036	10.741	1.00	11.64
ATOM	801	C7	SEI A 129	29.405	18.197	10.462	1.00	2.00
ATOM	802	C8	SEI A 129	31.769	15.900	5.468	1.00	5.88
ATOM	803	C9	SEI A 129	30.614	14.989	5.035	1.00	10.05
ATOM	804	C10	SEI A 129	33.106	15.201	5.285	1.00	10.92
ATOM	805	N	SEI A 129	30.916	22.193	6.024	1.00	7.00
ATOM	806	CA	SEI A 129	31.186	20.804	5.818	1.00	4.93
ATOM	807	C	SEI A 129	30.516	20.458	4.534	1.00	3.57
ATOM	808	O	SEI A 129	29.305	20.529	4.410	1.00	5.86
ATOM	809	CB	SEI A 129	30.536	20.063	6.956	1.00	4.94
ATOM	810	O2	SEI A 129	33.031	18.359	7.260	1.00	17.04
ATOM	811	N	LEU A 130	31.332	20.138	3.541	1.00	4.70
ATOM	812	CA	LEU A 130	30.814	19.774	2.219	1.00	6.09
ATOM	813	CB	LEU A 130	31.825	20.095	1.127	1.00	8.94
ATOM	814	CG	LEU A 130	31.491	19.566	-0.273	1.00	2.00
ATOM	815	CD1	LEU A 130	30.306	20.309	-0.854	1.00	2.00
ATOM	816	CD2	LEU A 130	32.720	19.745	-1.157	1.00	4.46
ATOM	817	C	LEU A 130	30.500	18.314	2.158	1.00	6.28
ATOM	818	O	LEU A 130	31.293	17.487	2.554	1.00	12.07
ATOM	819	N	SER A 131	29.320	17.984	1.669	1.00	8.28
ATOM	820	CA	SER A 131	28.978	16.564	1.504	1.00	8.85
ATOM	821	CB	SER A 131	27.618	16.283	2.096	1.00	5.12
ATOM	822	OG	SER A 131	27.656	16.625	3.465	1.00	19.47
ATOM	823	C	SER A 131	29.022	16.243	-0.003	1.00	10.39
ATOM	824	O	SER A 131	28.527	16.996	-0.846	1.00	11.22
ATOM	825	N	THR A 132	29.664	15.127	-0.333	1.00	12.55
ATOM	826	CA	THR A 132	29.790	14.670	-1.728	1.00	16.62
ATOM	827	CB	THR A 132	31.271	14.437	-2.085	1.00	15.84
ATOM	828	OG1	THR A 132	31.893	13.713	-1.019	1.00	16.85
ATOM	829	CG2	THR A 132	32.004	15.768	-2.282	1.00	14.99
ATOM	830	C	THR A 132	29.028	13.347	-1.849	1.00	19.10
ATOM	831	O	THR A 132	28.990	12.558	-0.903	1.00	18.44

Fig. 4Q

ATOM	832	N	ALA A 133	28.363	13.150	-2.992	1.00	24.92
ATOM	833	CA	ALA A 133	27.602	11.895	-3.254	1.00	30.53
ATOM	834	CB	ALA A 133	26.599	12.110	-4.378	1.00	28.49
ATOM	835	C	ALA A 133	28.612	10.768	-3.625	1.00	35.62
ATOM	836	O	ALA A 133	28.611	9.704	-2.964	1.00	42.46
ATOM	837	OT	ALA A 133	29.435	10.985	-4.541	1.00	39.35
ATOM	838	CB	ALA A 141	34.850	13.048	-10.291	1.00	40.89
ATOM	839	C	ALA A 141	32.972	13.033	-12.027	1.00	36.57
ATOM	840	O	ALA A 141	33.249	12.981	-13.225	1.00	35.01
ATOM	841	N	ALA A 141	34.375	11.021	-11.658	1.00	39.81
ATOM	842	CA	ALA A 141	33.753	12.194	-10.976	1.00	38.55
ATOM	843	N	ASP A 142	31.971	13.777	-11.564	1.00	35.82
ATOM	844	CA	ASP A 142	31.137	14.620	-12.475	1.00	37.99
ATOM	845	CB	ASP A 142	30.125	13.758	-13.231	1.00	41.81
ATOM	846	CG	ASP A 142	28.984	13.256	-12.345	1.00	46.15
ATOM	847	OD1	ASP A 142	27.863	13.801	-12.478	1.00	53.97
ATOM	848	OD2	ASP A 142	29.195	12.310	-11.547	1.00	46.27
ATOM	849	C	ASP A 142	30.433	15.767	-11.713	1.00	36.58
ATOM	850	O	ASP A 142	30.523	15.872	-10.493	1.00	38.92
ATOM	851	N	ARG A 143	29.686	16.588	-12.451	1.00	34.69
ATOM	852	CA	ARG A 143	28.973	17.779	-11.894	1.00	32.35
ATOM	853	CB	ARG A 143	28.284	18.540	-13.030	1.00	32.68
ATOM	854	CG	ARG A 143	29.038	18.581	-14.333	1.00	32.20
ATOM	855	CD	ARG A 143	29.532	19.965	-14.668	1.00	39.13
ATOM	856	NE	ARG A 143	29.940	20.069	-16.077	1.00	48.59
ATOM	857	CZ	ARG A 143	31.068	20.638	-16.510	1.00	50.60
ATOM	858	NH1	ARG A 143	31.324	20.687	-17.806	1.00	50.22
ATOM	859	NH2	ARG A 143	31.966	21.116	-15.660	1.00	54.07
ATOM	860	C	ARG A 143	27.970	17.539	-10.722	1.00	33.03
ATOM	861	O	ARG A 143	27.458	18.471	-10.110	1.00	35.26
ATOM	862	N	THR A 144	27.688	16.279	-10.415	1.00	31.99
ATOM	863	CA	THR A 144	26.751	15.942	-9.304	1.00	29.49
ATOM	864	CB	THR A 144	25.807	14.787	-9.716	1.00	31.98
ATOM	865	OG1	THR A 144	26.568	13.581	-9.877	1.00	33.87
ATOM	866	CG2	THR A 144	25.110	15.099	-11.040	1.00	35.59
ATOM	867	C	THR A 144	27.506	15.492	-8.023	1.00	27.75
ATOM	868	O	THR A 144	26.920	14.959	-7.075	1.00	30.96
ATOM	869	N	LEU A 145	28.823	15.680	-8.021	1.00	22.66
ATOM	870	CA	LEU A 145	29.661	15.264	-6.872	1.00	19.42
ATOM	871	CB	LEU A 145	31.138	15.419	-7.230	1.00	14.05
ATOM	872	CG	LEU A 145	32.091	14.911	-6.166	1.00	9.94
ATOM	873	CD1	LEU A 145	31.931	13.444	-5.988	1.00	6.47
ATOM	874	CD2	LEU A 145	33.492	15.243	-6.544	1.00	14.60
ATOM	875	C	LEU A 145	29.305	16.052	-5.584	1.00	19.44
ATOM	876	O	LEU A 145	29.122	15.493	-4.507	1.00	21.52
ATOM	877	N	PHE A 146	29.237	17.370	-5.709	1.00	13.66
ATOM	878	CA	PHE A 146	28.890	18.214	-4.566	1.00	13.40
ATOM	879	CB	PHE A 146	29.315	19.653	-4.849	1.00	11.02
ATOM	880	CG	PHE A 146	30.800	19.839	-4.893	1.00	4.61
ATOM	881	CD1	PHE A 146	31.338	21.086	-5.053	1.00	4.68
ATOM	882	CD2	PHE A 146	31.647	18.760	-4.774	1.00	4.07
ATOM	883	CE1	PHE A 146	32.699	21.250	-5.094	1.00	6.69

Fig. 4R

ATOM	884	CE2	PHE A 146	32.989	18.914	-4.815	1.00	2.42
ATOM	885	CZ	PHE A 146	33.527	20.150	-4.975	1.00	3.42
ATOM	886	C	PHE A 146	27.387	18.112	-4.267	1.00	14.49
ATOM	887	O	PHE A 146	26.542	18.509	-5.063	1.00	19.13
ATOM	888	N	ALA A 147	27.074	17.547	-3.101	1.00	13.64
ATOM	889	CA	ALA A 147	25.671	17.346	-2.640	1.00	10.83
ATOM	890	CB	ALA A 147	25.614	16.168	-1.715	1.00	9.08
ATOM	891	C	ALA A 147	25.084	18.593	-1.940	1.00	11.80
ATOM	892	O	ALA A 147	24.067	19.126	-2.341	1.00	15.54
ATOM	893	N	HIS A 148	25.733	19.031	-0.862	1.00	12.59
ATOM	894	CA	HIS A 148	25.300	20.234	-0.089	1.00	10.63
ATOM	895	CB	HIS A 148	23.987	19.958	0.619	1.00	10.37
ATOM	896	CG	HIS A 148	24.047	18.808	1.577	1.00	19.25
ATOM	897	CD2	HIS A 148	23.866	17.477	1.389	1.00	23.23
ATOM	898	ND1	HIS A 148	24.283	18.967	2.926	1.00	26.01
ATOM	899	CE1	HIS A 148	24.244	17.791	3.527	1.00	23.57
ATOM	900	NE2	HIS A 148	23.992	16.869	2.615	1.00	25.40
ATOM	901	C	HIS A 148	26.358	20.634	0.949	1.00	12.85
ATOM	902	O	HIS A 148	27.342	19.912	1.222	1.00	10.96
ATOM	903	N	VAL A 149	26.145	21.803	1.547	1.00	9.18
ATOM	904	CA	VAL A 149	27.067	22.274	2.595	1.00	7.72
ATOM	905	CB	VAL A 149	27.780	23.596	2.229	1.00	9.50
ATOM	906	CG1	VAL A 149	28.036	23.637	0.751	1.00	11.54
ATOM	907	CG2	VAL A 149	27.012	24.800	2.695	1.00	11.06
ATOM	908	C	VAL A 149	26.277	22.435	3.880	1.00	7.39
ATOM	909	O	VAL A 149	25.120	22.861	3.904	1.00	6.80
ATOM	910	N	ALA A 150	26.916	22.032	4.964	1.00	7.47
ATOM	911	CA	ALA A 150	26.302	22.093	6.270	1.00	5.81
ATOM	912	CB	ALA A 150	26.244	20.710	6.876	1.00	2.00
ATOM	913	C	ALA A 150	27.130	23.017	7.142	1.00	5.80
ATOM	914	O	ALA A 150	28.347	23.019	7.091	1.00	15.09
ATOM	915	N	LEU A 151	26.443	23.901	7.853	1.00	5.33
ATOM	916	CA	LEU A 151	27.083	24.817	8.800	1.00	3.39
ATOM	917	CB	LEU A 151	26.157	25.991	9.072	1.00	5.70
ATOM	918	CG	LEU A 151	26.241	27.301	8.296	1.00	7.34
ATOM	919	CD1	LEU A 151	26.854	27.107	6.939	1.00	3.41
ATOM	920	CD2	LEU A 151	24.841	27.925	8.241	1.00	4.66
ATOM	921	C	LEU A 151	27.204	23.934	10.043	1.00	3.49
ATOM	922	O	LEU A 151	26.316	23.128	10.340	1.00	2.65
ATOM	923	N	CYS A 152	28.306	24.058	10.770	1.00	5.06
ATOM	924	CA	CYS A 152	28.482	23.240	11.983	1.00	2.81
ATOM	925	CB	CYS A 152	28.884	21.838	11.561	1.00	2.00
ATOM	926	SG	CYS A 152	30.351	21.833	10.545	1.00	12.33
ATOM	927	C	CYS A 152	29.525	23.887	12.880	1.00	3.00
ATOM	928	O	CYS A 152	30.084	24.917	12.574	1.00	6.88
ATOM	929	N	ALA A 153	29.777	23.273	14.019	1.00	5.62
ATOM	930	CA	ALA A 153	30.765	23.806	14.978	1.00	5.99
ATOM	931	CB	ALA A 153	30.505	23.247	16.345	1.00	3.64
ATOM	932	C	ALA A 153	32.198	23.519	14.579	1.00	4.87
ATOM	933	O	ALA A 153	33.069	24.366	14.631	1.00	8.95
ATOM	934	N	ILE A 154	32.449	22.278	14.209	1.00	3.33
ATOM	935	CA	ILE A 154	33.791	21.856	13.831	1.00	6.57

Fig. 4S

ATOM	936	CB	ILE	A	154	34.519	21.214	15.065	1.00	13.23
ATOM	937	CG2	ILE	A	154	35.849	20.661	14.679	1.00	15.20
ATOM	938	CG1	ILE	A	154	34.742	22.247	16.184	1.00	17.08
ATOM	939	CD1	ILE	A	154	35.736	23.354	15.845	1.00	21.42
ATOM	940	C	ILE	A	154	33.620	20.837	12.671	1.00	8.07
ATOM	941	O	ILE	A	154	32.935	19.820	12.802	1.00	6.60
ATOM	942	N	GLY	A	155	34.206	21.179	11.516	1.00	7.25
ATOM	943	CA	GLY	A	155	34.138	20.338	10.335	1.00	8.29
ATOM	944	C	GLY	A	155	35.202	19.269	10.364	1.00	9.30
ATOM	945	O	GLY	A	155	36.071	19.289	11.239	1.00	11.83
ATOM	946	N	ARG	A	156	35.176	18.363	9.393	1.00	8.85
ATOM	947	CA	ARG	A	156	36.182	17.277	9.359	1.00	10.92
ATOM	948	CB	ARG	A	156	35.496	15.967	8.996	1.00	17.70
ATOM	949	CG	ARG	A	156	34.400	15.595	9.973	1.00	20.67
ATOM	950	CD	ARG	A	156	34.337	14.120	10.205	1.00	29.56
ATOM	951	NE	ARG	A	156	34.168	13.376	8.965	1.00	41.87
ATOM	952	CZ	ARG	A	156	34.645	12.149	8.765	1.00	50.41
ATOM	953	NH1	ARG	A	156	34.438	11.536	7.603	1.00	51.55
ATOM	954	NH2	ARG	A	156	35.340	11.537	9.724	1.00	54.89
ATOM	955	C	ARG	A	156	37.420	17.537	8.476	1.00	10.96
ATOM	956	O	ARG	A	156	38.466	16.913	8.597	1.00	13.19
ATOM	957	N	ARG	A	157	37.278	18.458	7.547	1.00	9.18
ATOM	958	CA	ARG	A	157	38.395	18.809	6.689	1.00	7.21
ATOM	959	CB	ARG	A	157	37.889	19.001	5.268	1.00	3.14
ATOM	960	CG	ARG	A	157	37.587	17.685	4.570	1.00	5.26
ATOM	961	CD	ARG	A	157	37.501	17.781	3.034	1.00	5.80
ATOM	962	NE	ARG	A	157	36.109	17.989	2.665	1.00	9.28
ATOM	963	CZ	ARG	A	157	35.294	17.125	2.068	1.00	10.11
ATOM	964	NH1	ARG	A	157	35.612	15.920	1.630	1.00	7.28
ATOM	965	NH2	ARG	A	157	34.036	17.269	2.355	1.00	17.52
ATOM	966	C	ARG	A	157	39.054	20.074	7.280	1.00	9.04
ATOM	967	O	ARG	A	157	38.454	20.808	8.066	1.00	7.54
ATOM	968	N	LEU	A	158	40.319	20.283	6.932	1.00	6.31
ATOM	969	CA	LEU	A	158	41.091	21.432	7.439	1.00	2.00
ATOM	970	CB	LEU	A	158	42.568	21.158	7.234	1.00	2.00
ATOM	971	CG	LEU	A	158	43.293	20.467	8.376	1.00	5.80
ATOM	972	CD1	LEU	A	158	42.343	19.641	9.242	1.00	6.29
ATOM	973	CD2	LEU	A	158	44.370	19.612	7.804	1.00	2.00
ATOM	974	C	LEU	A	158	40.711	22.761	6.823	1.00	5.67
ATOM	975	O	LEU	A	158	40.080	22.835	5.778	1.00	7.66
ATOM	976	N	GLY	A	159	41.160	23.830	7.473	1.00	5.29
ATOM	977	CA	GLY	A	159	40.894	25.173	7.002	1.00	6.28
ATOM	978	C	GLY	A	159	39.459	25.541	6.686	1.00	8.92
ATOM	979	O	GLY	A	159	39.219	26.610	6.096	1.00	12.32
ATOM	980	N	THR	A	160	38.503	24.739	7.154	1.00	3.52
ATOM	981	CA	THR	A	160	37.093	25.016	6.878	1.00	2.40
ATOM	982	CB	THR	A	160	36.277	23.746	6.799	1.00	4.71
ATOM	983	OG1	THR	A	160	36.602	22.888	7.903	1.00	2.00
ATOM	984	CG2	THR	A	160	36.540	23.050	5.480	1.00	2.00
ATOM	985	C	THR	A	160	36.412	25.949	7.837	1.00	4.22
ATOM	986	O	THR	A	160	35.346	25.662	8.349	1.00	7.62
ATOM	987	N	ILE	A	161	37.009	27.101	8.068	1.00	2.82

Fig. 4T

ATOM	988	CA	ILE A 161	36.397	28.064	8.963	1.00	3.28
ATOM	989	CB	ILE A 161	37.437	28.672	9.857	1.00	2.00
ATOM	990	CG2	ILE A 161	36.878	29.842	10.580	1.00	2.00
ATOM	991	CG1	ILE A 161	37.919	27.623	10.853	1.00	2.99
ATOM	992	CD1	ILE A 161	36.891	27.160	11.792	1.00	2.00
ATOM	993	C	ILE A 161	35.779	29.109	8.053	1.00	6.97
ATOM	994	O	ILE A 161	36.444	29.599	7.133	1.00	9.59
ATOM	995	N	VAL A 162	34.500	29.420	8.286	1.00	5.77
ATOM	996	CA	VAL A 162	33.770	30.408	7.447	1.00	5.15
ATOM	997	CB	VAL A 162	32.365	29.916	7.046	1.00	2.00
ATOM	998	CG1	VAL A 162	32.462	28.600	6.303	1.00	2.00
ATOM	999	CG2	VAL A 162	31.496	29.786	8.267	1.00	2.00
ATOM	1000	C	VAL A 162	33.646	31.801	8.078	1.00	7.04
ATOM	1001	O	VAL A 162	33.995	32.031	9.224	1.00	12.34
ATOM	1002	N	THR A 163	33.154	32.733	7.265	1.00	10.55
ATOM	1003	CA	THR A 163	32.935	34.153	7.619	1.00	5.79
ATOM	1004	CB	THR A 163	33.805	35.069	6.743	1.00	2.00
ATOM	1005	OG1	THR A 163	35.168	34.996	7.158	1.00	10.28
ATOM	1006	CG2	THR A 163	33.376	36.457	6.870	1.00	9.64
ATOM	1007	C	THR A 163	31.462	34.462	7.269	1.00	7.38
ATOM	1008	O	THR A 163	30.920	33.997	6.268	1.00	9.26
ATOM	1009	N	TYR A 164	30.828	35.273	8.104	1.00	6.43
ATOM	1010	CA	TYR A 164	29.425	35.671	7.910	1.00	2.00
ATOM	1011	CB	TYR A 164	28.555	35.167	9.057	1.00	5.35
ATOM	1012	CG	TYR A 164	28.398	33.674	9.212	1.00	3.93
ATOM	1013	CD1	TYR A 164	29.240	32.945	10.051	1.00	10.71
ATOM	1014	CE1	TYR A 164	29.039	31.590	10.263	1.00	3.10
ATOM	1015	CD2	TYR A 164	27.365	33.003	8.587	1.00	2.00
ATOM	1016	CE2	TYR A 164	27.163	31.656	8.794	1.00	2.00
ATOM	1017	CZ	TYR A 164	27.994	30.957	9.631	1.00	2.00
ATOM	1018	OH	TYR A 164	27.757	29.617	9.848	1.00	7.05
ATOM	1019	C	TYR A 164	29.350	37.181	7.918	1.00	2.77
ATOM	1020	O	TYR A 164	29.950	37.836	8.760	1.00	5.86
ATOM	1021	N	ASP A 165	28.603	37.754	6.991	1.00	3.90
ATOM	1022	CA	ASP A 165	28.437	39.221	6.997	1.00	5.48
ATOM	1023	CB	ASP A 165	29.675	39.950	6.514	1.00	6.87
ATOM	1024	CG	ASP A 165	29.963	41.194	7.343	1.00	6.94
ATOM	1025	OD1	ASP A 165	29.217	42.183	7.246	1.00	10.37
ATOM	1026	OD2	ASP A 165	30.935	41.186	8.112	1.00	13.48
ATOM	1027	C	ASP A 165	27.220	39.603	6.182	1.00	5.17
ATOM	1028	O	ASP A 165	26.632	38.767	5.512	1.00	10.46
ATOM	1029	N	THR A 166	26.805	40.860	6.288	1.00	2.54
ATOM	1030	CA	THR A 166	25.605	41.331	5.564	1.00	8.12
ATOM	1031	CB	THR A 166	24.839	42.392	6.361	1.00	8.39
ATOM	1032	OG1	THR A 166	25.734	43.462	6.710	1.00	7.48
ATOM	1033	CG2	THR A 166	24.245	41.778	7.612	1.00	3.71
ATOM	1034	C	THR A 166	25.901	41.883	4.171	1.00	9.37
ATOM	1035	O	THR A 166	25.077	42.532	3.532	1.00	11.11
ATOM	1036	N	SER A 167	27.116	41.645	3.704	1.00	9.87
ATOM	1037	CA	SER A 167	27.503	42.089	2.361	1.00	6.92
ATOM	1038	CB	SER A 167	28.132	43.460	2.430	1.00	8.33
ATOM	1039	OG	SER A 167	29.523	43.410	2.230	1.00	16.34

Fig. 4U

ATOM	1040	C	SER A 167	28.468	41.029	1.885	1.00	8.44
ATOM	1041	O	SER A 167	29.252	40.491	2.655	1.00	12.99
ATOM	1042	N	LEU A 168	28.379	40.676	0.611	1.00	8.80
ATOM	1043	CA	LEU A 168	29.280	39.636	0.069	1.00	10.94
ATOM	1044	CB	LEU A 168	28.897	39.309	-1.370	1.00	5.14
ATOM	1045	CG	LEU A 168	29.694	38.235	-2.092	1.00	3.65
ATOM	1046	CD1	LEU A 168	28.868	37.674	-3.190	1.00	13.15
ATOM	1047	CD2	LEU A 168	30.944	38.825	-2.696	1.00	16.58
ATOM	1048	C	LEU A 168	30.741	40.078	0.194	1.00	9.88
ATOM	1049	O	LEU A 168	31.588	39.384	0.724	1.00	15.05
ATOM	1050	N	ASP A 169	30.987	41.311	-0.219	1.00	12.69
ATOM	1051	CA	ASP A 169	32.339	41.918	-0.177	1.00	11.13
ATOM	1052	CB	ASP A 169	32.272	43.354	-0.694	1.00	10.36
ATOM	1053	CG	ASP A 169	32.399	43.443	-2.193	1.00	12.34
ATOM	1054	OD1	ASP A 169	32.686	44.547	-2.701	1.00	19.74
ATOM	1055	OD2	ASP A 169	32.227	42.423	-2.876	1.00	14.21
ATOM	1056	C	ASP A 169	32.948	41.873	1.225	1.00	10.65
ATOM	1057	O	ASP A 169	34.134	41.626	1.411	1.00	9.59
ATOM	1058	N	ALA A 170	32.095	42.098	2.221	1.00	10.94
ATOM	1059	CA	ALA A 170	32.530	42.107	3.633	1.00	7.86
ATOM	1060	CB	ALA A 170	31.515	42.782	4.477	1.00	12.83
ATOM	1061	C	ALA A 170	32.780	40.702	4.156	1.00	7.65
ATOM	1062	O	ALA A 170	33.551	40.492	5.081	1.00	10.44
ATOM	1063	N	ALA A 171	32.090	39.737	3.566	1.00	3.95
ATOM	1064	CA	ALA A 171	32.241	38.347	3.955	1.00	2.00
ATOM	1065	CB	ALA A 171	31.040	37.559	3.493	1.00	4.68
ATOM	1066	C	ALA A 171	33.536	37.766	3.354	1.00	5.20
ATOM	1067	O	ALA A 171	34.199	36.918	3.946	1.00	8.71
ATOM	1068	N	ILE A 172	33.904	38.215	2.158	1.00	4.62
ATOM	1069	CA	ILE A 172	35.138	37.689	1.538	1.00	7.44
ATOM	1070	CB	ILE A 172	35.016	37.510	-0.014	1.00	7.03
ATOM	1071	CG2	ILE A 172	33.634	37.052	-0.361	1.00	10.50
ATOM	1072	CG1	ILE A 172	35.273	38.802	-0.780	1.00	5.94
ATOM	1073	CD1	ILE A 172	35.114	38.641	-2.290	1.00	2.00
ATOM	1074	C	ILE A 172	36.432	38.434	1.909	1.00	6.82
ATOM	1075	O	ILE A 172	37.525	37.872	1.879	1.00	11.31
ATOM	1076	N	ALA A 173	36.296	39.685	2.326	1.00	6.16
ATOM	1077	CA	ALA A 173	37.472	40.531	2.709	1.00	5.51
ATOM	1078	CB	ALA A 173	37.022	41.903	3.147	1.00	7.11
ATOM	1079	C	ALA A 173	38.457	39.940	3.742	1.00	5.49
ATOM	1080	O	ALA A 173	39.651	40.219	3.693	1.00	10.38
ATOM	1081	N	PRO A 174	37.969	39.179	4.735	1.00	3.89
ATOM	1082	CD	PRO A 174	36.611	39.047	5.286	1.00	2.26
ATOM	1083	CA	PRO A 174	38.941	38.628	5.689	1.00	2.00
ATOM	1084	CB	PRO A 174	38.075	38.045	6.791	1.00	2.00
ATOM	1085	CG	PRO A 174	36.907	38.932	6.769	1.00	3.89
ATOM	1086	C	PRO A 174	39.786	37.536	5.074	1.00	2.00
ATOM	1087	O	PRO A 174	40.638	36.968	5.726	1.00	8.03
ATOM	1088	N	PHE A 175	39.487	37.172	3.835	1.00	2.90
ATOM	1089	CA	PHE A 175	40.278	36.139	3.159	1.00	6.14
ATOM	1090	CB	PHE A 175	39.376	35.292	2.295	1.00	6.27
ATOM	1091	CG	PHE A 175	38.504	34.388	3.084	1.00	4.47

Fig. 4v

ATOM	1092	CD1	PHE	A	175	38.954	33.114	3.433	1.00	2.00
ATOM	1093	CD2	PHE	A	175	37.256	34.823	3.533	1.00	3.94
ATOM	1094	CE1	PHE	A	175	38.186	32.287	4.216	1.00	2.00
ATOM	1095	CE2	PHE	A	175	36.465	34.004	4.323	1.00	3.94
ATOM	1096	CZ	PHE	A	175	36.933	32.722	4.669	1.00	3.73
ATOM	1097	C	PHE	A	175	41.380	36.809	2.365	1.00	9.75
ATOM	1098	O	PHE	A	175	41.177	37.353	1.288	1.00	10.92
ATOM	1099	N	ARG	A	176	42.559	36.816	2.977	1.00	13.95
ATOM	1100	CA	ARG	A	176	43.751	37.439	2.400	1.00	12.43
ATOM	1101	CB	ARG	A	176	44.627	37.929	3.533	1.00	8.86
ATOM	1102	CG	ARG	A	176	43.912	38.821	4.513	1.00	9.09
ATOM	1103	CD	ARG	A	176	43.539	40.149	3.916	1.00	13.20
ATOM	1104	NE	ARG	A	176	42.418	40.731	4.644	1.00	17.45
ATOM	1105	CZ	ARG	A	176	42.535	41.620	5.624	1.00	16.50
ATOM	1106	NH1	ARG	A	176	41.463	42.094	6.247	1.00	16.11
ATOM	1107	NH2	ARG	A	176	43.718	42.063	5.960	1.00	12.86
ATOM	1108	C	ARG	A	176	44.543	36.532	1.441	1.00	18.03
ATOM	1109	O	ARG	A	176	45.286	36.994	0.587	1.00	21.73
ATOM	1110	N	HIS	A	177	44.426	35.221	1.595	1.00	21.39
ATOM	1111	CA	HIS	A	177	45.171	34.323	0.672	1.00	25.17
ATOM	1112	CB	HIS	A	177	45.790	33.156	1.429	1.00	33.05
ATOM	1113	CG	HIS	A	177	46.738	33.579	2.506	1.00	44.14
ATOM	1114	CD2	HIS	A	177	47.160	32.935	3.623	1.00	48.92
ATOM	1115	ND1	HIS	A	177	47.348	34.817	2.522	1.00	45.03
ATOM	1116	CE1	HIS	A	177	48.098	34.923	3.601	1.00	47.09
ATOM	1117	NE2	HIS	A	177	48.005	33.796	4.287	1.00	50.79
ATOM	1118	C	HIS	A	177	44.203	33.831	-0.391	1.00	25.38
ATOM	1119	O	HIS	A	177	43.909	32.648	-0.520	1.00	28.71
ATOM	1120	N	LEU	A	178	43.681	34.780	-1.154	1.00	23.91
ATOM	1121	CA	LEU	A	178	42.701	34.468	-2.211	1.00	22.54
ATOM	1122	CB	LEU	A	178	41.331	34.999	-1.795	1.00	19.32
ATOM	1123	CG	LEU	A	178	40.121	34.072	-1.941	1.00	17.09
ATOM	1124	CD1	LEU	A	178	40.298	32.847	-1.069	1.00	11.07
ATOM	1125	CD2	LEU	A	178	38.874	34.820	-1.536	1.00	9.82
ATOM	1126	C	LEU	A	178	43.127	35.049	-3.570	1.00	23.94
ATOM	1127	O	LEU	A	178	43.453	36.226	-3.731	1.00	29.67
ATOM	1128	N	ASP	A	179	43.163	34.178	-4.562	1.00	21.90
ATOM	1129	CA	ASP	A	179	43.534	34.603	-5.903	1.00	19.53
ATOM	1130	CB	ASP	A	179	43.448	33.410	-6.835	1.00	20.21
ATOM	1131	CG	ASP	A	179	44.181	33.619	-8.116	1.00	19.59
ATOM	1132	OD1	ASP	A	179	43.783	34.499	-8.900	1.00	16.37
ATOM	1133	OD2	ASP	A	179	45.153	32.883	-8.345	1.00	23.15
ATOM	1134	C	ASP	A	179	42.553	35.719	-6.307	1.00	24.43
ATOM	1135	O	ASP	A	179	41.355	35.691	-6.008	1.00	22.22
ATOM	1136	N	PRO	A	180	43.084	36.763	-6.957	1.00	27.44
ATOM	1137	CD	PRO	A	180	44.521	36.981	-7.209	1.00	26.55
ATOM	1138	CA	PRO	A	180	42.299	37.908	-7.420	1.00	24.01
ATOM	1139	CB	PRO	A	180	43.327	38.702	-8.202	1.00	24.07
ATOM	1140	CG	PRO	A	180	44.575	38.455	-7.419	1.00	26.33
ATOM	1141	C	PRO	A	180	41.152	37.461	-8.330	1.00	22.37
ATOM	1142	O	PRO	A	180	40.064	38.011	-8.321	1.00	26.56
ATOM	1143	N	ALA	A	181	41.421	36.444	-9.138	1.00	20.29

Fig. 4W

ATOM	1144	CA	ALA A 181	40.403	35.897	-10.058	1.00	19.95
ATOM	1145	CB	ALA A 181	40.999	34.814	-10.920	1.00	20.81
ATOM	1146	C	ALA A 181	39.229	35.329	-9.269	1.00	18.58
ATOM	1147	O	ALA A 181	38.070	35.541	-9.593	1.00	25.43
ATOM	1148	N	THR A 182	39.538	34.601	-8.208	1.00	14.88
ATOM	1149	CA	THR A 182	38.484	34.012	-7.376	1.00	14.96
ATOM	1150	CB	THR A 182	39.067	33.282	-6.198	1.00	12.63
ATOM	1151	OG1	THR A 182	40.015	32.324	-6.688	1.00	4.87
ATOM	1152	CG2	THR A 182	37.961	32.559	-5.423	1.00	7.24
ATOM	1153	C	THR A 182	37.515	35.083	-6.893	1.00	16.50
ATOM	1154	O	THR A 182	36.296	34.960	-7.015	1.00	16.74
ATOM	1155	N	ARG A 183	38.083	36.171	-6.387	1.00	15.79
ATOM	1156	CA	ARG A 183	37.271	37.290	-5.909	1.00	16.39
ATOM	1157	CB	ARG A 183	38.162	38.392	-5.392	1.00	13.25
ATOM	1158	CG	ARG A 183	38.990	37.955	-4.291	1.00	12.26
ATOM	1159	CD	ARG A 183	39.787	39.094	-3.834	1.00	25.61
ATOM	1160	NE	ARG A 183	40.577	38.678	-2.690	1.00	47.35
ATOM	1161	CZ	ARG A 183	41.857	38.984	-2.511	1.00	55.77
ATOM	1162	NH1	ARG A 183	42.493	38.548	-1.424	1.00	58.95
ATOM	1163	NH2	ARG A 183	42.494	39.723	-3.416	1.00	61.87
ATOM	1164	C	ARG A 183	36.375	37.823	-7.015	1.00	17.57
ATOM	1165	O	ARG A 183	35.167	37.929	-6.874	1.00	22.70
ATOM	1166	N	GLU A 184	36.980	38.144	-8.142	1.00	20.09
ATOM	1167	CA	GLU A 184	36.204	38.694	-9.272	1.00	26.95
ATOM	1168	CB	GLU A 184	37.170	39.212	-10.346	1.00	33.24
ATOM	1169	CG	GLU A 184	36.588	40.359	-11.193	1.00	46.75
ATOM	1170	CD	GLU A 184	35.811	41.419	-10.362	1.00	51.03
ATOM	1171	OE1	GLU A 184	36.437	42.126	-9.535	1.00	47.53
ATOM	1172	OE2	GLU A 184	34.570	41.544	-10.547	1.00	51.44
ATOM	1173	C	GLU A 184	35.146	37.720	-9.860	1.00	21.35
ATOM	1174	O	GLU A 184	34.106	38.106	-10.393	1.00	20.09
ATOM	1175	N	GLY A 185	35.402	36.437	-9.690	1.00	16.92
ATOM	1176	CA	GLY A 185	34.488	35.450	-10.216	1.00	15.65
ATOM	1177	C	GLY A 185	33.372	35.135	-9.256	1.00	14.47
ATOM	1178	O	GLY A 185	32.233	34.941	-9.653	1.00	12.70
ATOM	1179	N	VAL A 186	33.695	35.127	-7.974	1.00	15.32
ATOM	1180	CA	VAL A 186	32.705	34.802	-6.938	1.00	16.00
ATOM	1181	CB	VAL A 186	33.391	34.447	-5.609	1.00	14.82
ATOM	1182	CG1	VAL A 186	33.689	35.677	-4.794	1.00	15.65
ATOM	1183	CG2	VAL A 186	32.558	33.483	-4.874	1.00	13.63
ATOM	1184	C	VAL A 186	31.690	35.929	-6.756	1.00	15.03
ATOM	1185	O	VAL A 186	30.565	35.732	-6.307	1.00	13.19
ATOM	1186	N	ARG A 187	32.118	37.132	-7.117	1.00	14.81
ATOM	1187	CA	ARG A 187	31.253	38.326	-7.039	1.00	17.48
ATOM	1188	CB	ARG A 187	32.085	39.592	-7.084	1.00	12.71
ATOM	1189	CG	ARG A 187	32.845	39.920	-5.837	1.00	17.80
ATOM	1190	CD	ARG A 187	33.473	41.298	-5.983	1.00	16.35
ATOM	1191	NE	ARG A 187	34.205	41.709	-4.791	1.00	18.26
ATOM	1192	CZ	ARG A 187	35.517	41.941	-4.753	1.00	19.23
ATOM	1193	NH1	ARG A 187	36.091	42.308	-3.616	1.00	18.29
ATOM	1194	NH2	ARG A 187	36.263	41.794	-5.838	1.00	16.42
ATOM	1195	C	ARG A 187	30.266	38.337	-8.226	1.00	23.14

Fig. 4X

ATOM	1196	O	ARG A 187	29.100	38.725	-8.118	1.00	26.11
ATOM	1197	N	ARG A 188	30.787	37.940	-9.383	1.00	23.78
ATOM	1198	CA	ARG A 188	30.015	37.897	-10.636	1.00	22.60
ATOM	1199	CB	ARG A 188	30.970	37.659	-11.809	1.00	27.05
ATOM	1200	CG	ARG A 188	30.412	38.067	-13.169	1.00	36.79
ATOM	1201	CD	ARG A 188	30.536	36.945	-14.192	1.00	42.25
ATOM	1202	NE	ARG A 188	31.880	36.380	-14.186	1.00	53.44
ATOM	1203	CZ	ARG A 188	32.157	35.077	-14.147	1.00	58.14
ATOM	1204	NH1	ARG A 188	33.424	34.675	-14.135	1.00	62.47
ATOM	1205	NH2	ARG A 188	31.178	34.175	-14.129	1.00	60.10
ATOM	1206	C	ARG A 188	28.934	36.817	-10.561	1.00	17.88
ATOM	1207	O	ARG A 188	27.764	37.070	-10.744	1.00	18.25
ATOM	1208	N	GLU A 189	29.341	35.599	-10.253	1.00	16.74
ATOM	1209	CA	GLU A 189	28.384	34.507	-10.154	1.00	16.68
ATOM	1210	CB	GLU A 189	29.102	33.198	-9.889	1.00	20.29
ATOM	1211	CG	GLU A 189	30.013	32.735	-11.008	1.00	30.56
ATOM	1212	CD	GLU A 189	30.724	31.427	-10.676	1.00	35.90
ATOM	1213	OE1	GLU A 189	31.854	31.221	-11.186	1.00	36.83
ATOM	1214	OE2	GLU A 189	30.163	30.616	-9.896	1.00	34.40
ATOM	1215	C	GLU A 189	27.348	34.772	-9.068	1.00	17.17
ATOM	1216	O	GLU A 189	26.152	34.669	-9.286	1.00	20.31
ATOM	1217	N	ALA A 190	27.818	35.165	-7.890	1.00	18.80
ATOM	1218	CA	ALA A 190	26.915	35.420	-6.730	1.00	17.03
ATOM	1219	CB	ALA A 190	27.716	35.814	-5.526	1.00	8.57
ATOM	1220	C	ALA A 190	25.779	36.434	-6.996	1.00	18.28
ATOM	1221	O	ALA A 190	24.653	36.283	-6.512	1.00	22.32
ATOM	1222	N	ALA A 191	26.078	37.460	-7.786	1.00	15.88
ATOM	1223	CA	ALA A 191	25.068	38.496	-8.136	1.00	17.67
ATOM	1224	CB	ALA A 191	25.735	39.624	-8.827	1.00	17.65
ATOM	1225	C	ALA A 191	23.951	37.923	-9.044	1.00	22.08
ATOM	1226	O	ALA A 191	22.757	38.224	-8.918	1.00	19.90
ATOM	1227	N	GLU A 192	24.376	37.129	-10.020	1.00	22.14
ATOM	1228	CA	GLU A 192	23.431	36.504	-10.935	1.00	24.00
ATOM	1229	CB	GLU A 192	24.170	35.797	-12.060	1.00	32.01
ATOM	1230	CG	GLU A 192	24.990	36.720	-12.955	1.00	43.84
ATOM	1231	CD	GLU A 192	25.704	35.981	-14.100	1.00	53.54
ATOM	1232	OE1	GLU A 192	25.543	34.735	-14.237	1.00	54.40
ATOM	1233	OE2	GLU A 192	26.434	36.661	-14.868	1.00	57.99
ATOM	1234	C	GLU A 192	22.591	35.525	-10.139	1.00	22.11
ATOM	1235	O	GLU A 192	21.383	35.623	-10.072	1.00	22.31
ATOM	1236	N	ALA A 193	23.275	34.602	-9.475	1.00	23.96
ATOM	1237	CA	ALA A 193	22.627	33.558	-8.647	1.00	21.81
ATOM	1238	CB	ALA A 193	23.647	32.818	-7.840	1.00	23.12
ATOM	1239	C	ALA A 193	21.587	34.165	-7.724	1.00	24.47
ATOM	1240	O	ALA A 193	20.495	33.629	-7.541	1.00	27.41
ATOM	1241	N	GLU A 194	21.932	35.300	-7.135	1.00	22.78
ATOM	1242	CA	GLU A 194	20.998	35.976	-6.241	1.00	26.02
ATOM	1243	CB	GLU A 194	21.637	37.184	-5.622	1.00	25.96
ATOM	1244	CG	GLU A 194	22.436	36.883	-4.434	1.00	27.36
ATOM	1245	CD	GLU A 194	22.890	38.142	-3.798	1.00	30.91
ATOM	1246	OE1	GLU A 194	24.048	38.553	-4.057	1.00	31.62
ATOM	1247	OE2	GLU A 194	22.067	38.738	-3.072	1.00	34.95

Fig. 4Y

ATOM	1248	C	GLU A 194	19.711	36.385	-6.923	1.00	26.18
ATOM	1249	O	GLU A 194	18.640	36.351	-6.343	1.00	28.88
ATOM	1250	N	LEU A 195	19.838	36.835	-8.161	1.00	28.13
ATOM	1251	CA	LEU A 195	18.672	37.258	-8.948	1.00	29.16
ATOM	1252	CB	LEU A 195	19.115	37.635	-10.348	1.00	32.65
ATOM	1253	CG	LEU A 195	19.854	38.959	-10.383	1.00	32.33
ATOM	1254	CD1	LEU A 195	20.238	39.320	-11.794	1.00	29.08
ATOM	1255	CD2	LEU A 195	18.918	39.999	-9.807	1.00	34.11
ATOM	1256	C	LEU A 195	17.584	36.196	-8.996	1.00	32.23
ATOM	1257	O	LEU A 195	16.397	36.495	-8.957	1.00	36.13
ATOM	1258	N	ALA A 196	18.003	34.942	-9.127	1.00	32.09
ATOM	1259	CA	ALA A 196	17.049	33.827	-9.159	1.00	37.21
ATOM	1260	CB	ALA A 196	17.772	32.532	-9.474	1.00	37.75
ATOM	1261	C	ALA A 196	16.344	33.733	-7.789	1.00	41.34
ATOM	1262	O	ALA A 196	15.216	34.183	-7.595	1.00	46.80
ATOM	1263	N	LEU A 197	17.058	33.213	-6.797	1.00	46.39
ATOM	1264	CA	LEU A 197	16.463	33.054	-5.441	1.00	48.16
ATOM	1265	CB	LEU A 197	17.284	32.052	-4.582	1.00	42.63
ATOM	1266	CG	LEU A 197	18.689	32.259	-4.007	1.00	40.14
ATOM	1267	CD1	LEU A 197	19.440	33.207	-4.874	1.00	43.51
ATOM	1268	CD2	LEU A 197	18.638	32.798	-2.592	1.00	43.15
ATOM	1269	C	LEU A 197	16.277	34.401	-4.750	1.00	48.97
ATOM	1270	O	LEU A 197	16.339	34.526	-3.526	1.00	54.40
ATOM	1271	N	ALA A 198	16.035	35.427	-5.558	1.00	48.46
ATOM	1272	CA	ALA A 198	15.839	36.779	-5.021	1.00	46.50
ATOM	1273	CB	ALA A 198	15.861	37.815	-6.127	1.00	51.57
ATOM	1274	C	ALA A 198	14.495	36.750	-4.361	1.00	41.42
ATOM	1275	O	ALA A 198	13.485	36.388	-4.944	1.00	39.01
ATOM	1276	N	GLY A 199	14.522	37.050	-3.075	1.00	40.95
ATOM	1277	CA	GLY A 199	13.307	37.066	-2.294	1.00	37.49
ATOM	1278	C	GLY A 199	13.098	35.783	-1.508	1.00	34.67
ATOM	1279	O	GLY A 199	12.342	35.774	-0.534	1.00	39.92
ATOM	1280	N	ARG A 200	13.740	34.693	-1.910	1.00	23.52
ATOM	1281	CA	ARG A 200	13.547	33.463	-1.170	1.00	15.36
ATOM	1282	CB	ARG A 200	14.187	32.302	-1.882	1.00	11.05
ATOM	1283	CG	ARG A 200	13.206	31.227	-2.159	1.00	14.32
ATOM	1284	CD	ARG A 200	13.514	29.972	-1.381	1.00	15.70
ATOM	1285	NE	ARG A 200	13.964	28.919	-2.284	1.00	21.84
ATOM	1286	CZ	ARG A 200	14.077	27.641	-1.945	1.00	26.11
ATOM	1287	NH1	ARG A 200	14.488	26.752	-2.842	1.00	28.82
ATOM	1288	NH2	ARG A 200	13.800	27.251	-0.707	1.00	27.00
ATOM	1289	C	ARG A 200	14.066	33.566	0.259	1.00	17.46
ATOM	1290	O	ARG A 200	15.121	34.141	0.560	1.00	16.43
ATOM	1291	N	THR A 201	13.237	33.036	1.149	1.00	15.44
ATOM	1292	CA	THR A 201	13.495	32.961	2.579	1.00	13.41
ATOM	1293	CB	THR A 201	12.463	33.751	3.352	1.00	16.83
ATOM	1294	OG1	THR A 201	12.586	35.117	2.968	1.00	29.43
ATOM	1295	CG2	THR A 201	12.696	33.632	4.889	1.00	21.71
ATOM	1296	C	THR A 201	13.251	31.505	2.872	1.00	13.79
ATOM	1297	O	THR A 201	12.439	30.847	2.216	1.00	15.67
ATOM	1298	N	TRP A 202	13.991	30.974	3.831	1.00	8.16
ATOM	1299	CA	TRP A 202	13.807	29.592	4.212	1.00	3.30

Fig. 42

ATOM	1300	CB	TRP A 202	15.174	28.925	4.296	1.00	4.64
ATOM	1301	CG	TRP A 202	15.771	28.616	2.922	1.00	4.90
ATOM	1302	CD2	TRP A 202	16.350	29.554	1.992	1.00	2.00
ATOM	1303	CE2	TRP A 202	16.708	28.829	0.835	1.00	2.00
ATOM	1304	CE3	TRP A 202	16.599	30.922	2.026	1.00	2.00
ATOM	1305	CD1	TRP A 202	15.821	27.389	2.306	1.00	2.00
ATOM	1306	NE1	TRP A 202	16.376	27.517	1.049	1.00	3.02
ATOM	1307	CZ2	TRP A 202	17.295	29.433	-0.269	1.00	5.31
ATOM	1308	CZ3	TRP A 202	17.185	31.520	0.927	1.00	2.00
ATOM	1309	CH2	TRP A 202	17.525	30.780	-0.205	1.00	2.00
ATOM	1310	C	TRP A 202	13.065	29.639	5.538	1.00	3.53
ATOM	1311	O	TRP A 202	13.029	30.653	6.208	1.00	9.14
ATOM	1312	N	ALA A 203	12.376	28.567	5.880	1.00	5.19
ATOM	1313	CA	ALA A 203	11.643	28.526	7.170	1.00	2.52
ATOM	1314	CB	ALA A 203	10.311	29.159	7.025	1.00	3.82
ATOM	1315	C	ALA A 203	11.501	27.061	7.568	1.00	6.65
ATOM	1316	O	ALA A 203	10.440	26.446	7.473	1.00	8.95
ATOM	1317	N	PRO A 204	12.608	26.469	8.041	1.00	9.57
ATOM	1318	CD	PRO A 204	13.938	27.091	8.172	1.00	6.21
ATOM	1319	CA	PRO A 204	12.651	25.062	8.455	1.00	8.75
ATOM	1320	CB	PRO A 204	14.153	24.833	8.689	1.00	3.21
ATOM	1321	CG	PRO A 204	14.642	26.156	9.094	1.00	3.99
ATOM	1322	C	PRO A 204	11.763	24.635	9.647	1.00	8.59
ATOM	1323	O	PRO A 204	11.392	23.465	9.781	1.00	12.31
ATOM	1324	N	GLY A 205	11.395	25.608	10.482	1.00	8.27
ATOM	1325	CA	GLY A 205	10.571	25.347	11.649	1.00	3.11
ATOM	1326	C	GLY A 205	11.370	25.669	12.896	1.00	5.42
ATOM	1327	O	GLY A 205	12.368	25.009	13.143	1.00	9.36
ATOM	1328	N	VAL A 206	10.917	26.619	13.721	1.00	6.38
ATOM	1329	CA	VAL A 206	11.685	27.008	14.914	1.00	6.22
ATOM	1330	CB	VAL A 206	11.080	28.207	15.710	1.00	6.22
ATOM	1331	CG1	VAL A 206	10.724	29.351	14.784	1.00	2.24
ATOM	1332	CG2	VAL A 206	9.927	27.801	16.496	1.00	9.41
ATOM	1333	C	VAL A 206	12.023	25.841	15.819	1.00	11.28
ATOM	1334	O	VAL A 206	13.141	25.729	16.314	1.00	13.84
ATOM	1335	N	GLU A 207	11.091	24.913	15.989	1.00	10.07
ATOM	1336	CA	GLU A 207	11.417	23.764	16.847	1.00	13.64
ATOM	1337	CB	GLU A 207	10.180	22.955	17.213	1.00	19.55
ATOM	1338	CG	GLU A 207	9.265	23.633	18.231	1.00	27.99
ATOM	1339	CD	GLU A 207	10.000	24.472	19.286	1.00	33.29
ATOM	1340	OE1	GLU A 207	11.063	24.067	19.806	1.00	35.11
ATOM	1341	OE2	GLU A 207	9.492	25.565	19.605	1.00	38.85
ATOM	1342	C	GLU A 207	12.477	22.878	16.209	1.00	13.37
ATOM	1343	O	GLU A 207	13.373	22.371	16.876	1.00	16.43
ATOM	1344	N	ALA A 208	12.362	22.694	14.895	1.00	10.76
ATOM	1345	CA	ALA A 208	13.336	21.884	14.132	1.00	7.80
ATOM	1346	CB	ALA A 208	13.002	21.900	12.670	1.00	3.93
ATOM	1347	C	ALA A 208	14.690	22.561	14.349	1.00	11.06
ATOM	1348	O	ALA A 208	15.686	21.944	14.711	1.00	9.59
ATOM	1349	N	LEU A 209	14.681	23.880	14.190	1.00	9.05
ATOM	1350	CA	LEU A 209	15.889	24.673	14.368	1.00	7.77
ATOM	1351	CB	LEU A 209	15.606	26.121	14.040	1.00	5.75

Fig. 4AA

ATOM	1352	CG	LEU	A	209	15.872	26.381	12.570	1.00	5.74
ATOM	1353	CD1	LEU	A	209	15.452	27.779	12.183	1.00	4.57
ATOM	1354	CD2	LEU	A	209	17.336	26.151	12.332	1.00	4.67
ATOM	1355	C	LEU	A	209	16.428	24.550	15.774	1.00	8.89
ATOM	1356	O	LEU	A	209	17.611	24.337	16.014	1.00	10.17
ATOM	1357	N	THR	A	210	15.517	24.652	16.723	1.00	8.02
ATOM	1358	CA	THR	A	210	15.895	24.594	18.127	1.00	7.75
ATOM	1359	CB	THR	A	210	14.663	24.882	19.023	1.00	11.59
ATOM	1360	OG1	THR	A	210	14.240	26.240	18.823	1.00	13.82
ATOM	1361	CG2	THR	A	210	14.994	24.705	20.471	1.00	9.00
ATOM	1362	C	THR	A	210	16.537	23.243	18.462	1.00	7.25
ATOM	1363	O	THR	A	210	17.602	23.159	19.047	1.00	2.23
ATOM	1364	N	HIS	A	211	15.899	22.169	18.017	1.00	13.28
ATOM	1365	CA	HIS	A	211	16.410	20.814	18.306	1.00	14.39
ATOM	1366	CB	HIS	A	211	15.356	19.743	17.939	1.00	24.21
ATOM	1367	CG	HIS	A	211	14.163	19.719	18.861	1.00	32.10
ATOM	1368	CD2	HIS	A	211	13.060	20.508	18.916	1.00	35.49
ATOM	1369	ND1	HIS	A	211	14.028	18.810	19.891	1.00	36.32
ATOM	1370	CE1	HIS	A	211	12.901	19.037	20.539	1.00	38.59
ATOM	1371	NE2	HIS	A	211	12.295	20.061	19.968	1.00	39.12
ATOM	1372	C	HIS	A	211	17.749	20.577	17.621	1.00	12.30
ATOM	1373	O	HIS	A	211	18.697	20.066	18.224	1.00	17.25
ATOM	1374	N	THR	A	212	17.859	21.032	16.375	1.00	10.09
ATOM	1375	CA	THR	A	212	19.110	20.854	15.574	1.00	8.92
ATOM	1376	CB	THR	A	212	18.900	21.301	14.089	1.00	7.09
ATOM	1377	OG1	THR	A	212	18.004	20.392	13.449	1.00	8.35
ATOM	1378	CG2	THR	A	212	20.172	21.260	13.309	1.00	6.60
ATOM	1379	C	THR	A	212	20.352	21.537	16.219	1.00	9.02
ATOM	1380	O	THR	A	212	21.459	21.000	16.254	1.00	8.89
ATOM	1381	N	LEU	A	213	20.142	22.731	16.752	1.00	6.24
ATOM	1382	CA	LEU	A	213	21.203	23.459	17.414	1.00	2.00
ATOM	1383	CB	LEU	A	213	20.805	24.900	17.499	1.00	2.00
ATOM	1384	CG	LEU	A	213	20.712	25.597	16.140	1.00	2.00
ATOM	1385	CD1	LEU	A	213	20.216	27.028	16.362	1.00	2.00
ATOM	1386	CD2	LEU	A	213	22.055	25.630	15.448	1.00	2.00
ATOM	1387	C	LEU	A	213	21.574	22.854	18.802	1.00	6.60
ATOM	1388	O	LEU	A	213	22.729	22.862	19.238	1.00	8.97
ATOM	1389	N	LEU	A	214	20.597	22.267	19.480	1.00	7.27
ATOM	1390	CA	LEU	A	214	20.871	21.638	20.784	1.00	3.30
ATOM	1391	CB	LEU	A	214	19.593	21.107	21.396	1.00	6.48
ATOM	1392	CG	LEU	A	214	19.511	20.950	22.908	1.00	10.06
ATOM	1393	CD1	LEU	A	214	18.657	19.758	23.193	1.00	10.04
ATOM	1394	CD2	LEU	A	214	20.870	20.767	23.548	1.00	16.50
ATOM	1395	C	LEU	A	214	21.794	20.486	20.428	1.00	6.10
ATOM	1396	O	LEU	A	214	22.811	20.241	21.041	1.00	9.00
ATOM	1397	N	SER	A	215	21.401	19.760	19.393	1.00	9.89
ATOM	1398	CA	SER	A	215	22.193	18.594	18.867	1.00	10.91
ATOM	1399	CB	SER	A	215	21.475	18.029	17.639	1.00	12.69
ATOM	1400	OG	SER	A	215	22.031	16.804	17.213	1.00	12.85
ATOM	1401	C	SER	A	215	23.662	18.996	18.516	1.00	7.44
ATOM	1402	O	SER	A	215	24.631	18.285	18.772	1.00	4.85
ATOM	1403	N	THR	A	216	23.814	20.157	17.897	1.00	8.11

Fig. 4BB

ATOM	1404	CA	THR A 216	25.161	20.668	17.556	1.00	6.87
ATOM	1405	CB	THR A 216	25.051	22.047	16.856	1.00	7.00
ATOM	1406	OG1	THR A 216	24.446	21.878	15.569	1.00	15.03
ATOM	1407	CG2	THR A 216	26.413	22.705	16.672	1.00	4.75
ATOM	1408	C	THR A 216	26.007	20.800	18.869	1.00	13.37
ATOM	1409	O	THR A 216	27.191	20.500	18.921	1.00	17.43
ATOM	1410	N	ALA A 217	25.361	21.229	19.947	1.00	11.63
ATOM	1411	CA	ALA A 217	26.035	21.391	21.237	1.00	6.33
ATOM	1412	CB	ALA A 217	25.193	22.266	22.163	1.00	6.15
ATOM	1413	C	ALA A 217	26.286	20.035	21.901	1.00	8.61
ATOM	1414	O	ALA A 217	27.399	19.685	22.259	1.00	9.44
ATOM	1415	N	VAL A 218	25.223	19.255	22.054	1.00	9.17
ATOM	1416	CA	VAL A 218	25.338	17.961	22.734	1.00	8.52
ATOM	1417	CB	VAL A 218	23.982	17.252	22.852	1.00	3.62
ATOM	1418	CG1	VAL A 218	24.189	15.816	23.241	1.00	2.00
ATOM	1419	CG2	VAL A 218	23.134	17.950	23.920	1.00	2.00
ATOM	1420	C	VAL A 218	26.384	17.059	22.094	1.00	11.66
ATOM	1421	O	VAL A 218	27.199	16.438	22.754	1.00	16.46
ATOM	1422	N	ASN A 219	26.413	17.052	20.777	1.00	14.73
ATOM	1423	CA	ASN A 219	27.377	16.202	20.061	1.00	15.26
ATOM	1424	CB	ASN A 219	26.907	15.979	18.639	1.00	13.84
ATOM	1425	CG	ASN A 219	25.812	15.002	18.559	1.00	16.76
ATOM	1426	OD1	ASN A 219	25.936	13.857	19.009	1.00	19.12
ATOM	1427	ND2	ASN A 219	24.700	15.437	17.990	1.00	29.15
ATOM	1428	C	ASN A 219	28.838	16.686	20.051	1.00	15.41
ATOM	1429	O	ASN A 219	29.753	15.985	19.628	1.00	10.84
ATOM	1430	N	ASN A 220	29.047	17.917	20.484	1.00	15.22
ATOM	1431	CA	ASN A 220	30.400	18.469	20.507	1.00	15.52
ATOM	1432	CB	ASN A 220	30.474	19.727	19.646	1.00	18.98
ATOM	1433	CG	ASN A 220	30.445	19.430	18.158	1.00	19.48
ATOM	1434	OD1	ASN A 220	31.489	19.182	17.541	1.00	18.11
ATOM	1435	ND2	ASN A 220	29.248	19.477	17.565	1.00	19.30
ATOM	1436	C	ASN A 220	30.860	18.789	21.921	1.00	18.26
ATOM	1437	O	ASN A 220	31.887	19.443	22.122	1.00	21.04
ATOM	1438	N	MET A 221	30.104	18.312	22.908	1.00	20.02
ATOM	1439	CA	MET A 221	30.424	18.590	24.340	1.00	18.92
ATOM	1440	CB	MET A 221	29.282	18.146	25.246	1.00	14.70
ATOM	1441	CG	MET A 221	29.066	16.672	25.254	1.00	7.03
ATOM	1442	SD	MET A 221	27.847	16.303	26.412	1.00	15.09
ATOM	1443	CE	MET A 221	27.200	14.801	25.801	1.00	5.24
ATOM	1444	C	MET A 221	31.732	17.958	24.781	1.00	20.99
ATOM	1445	O	MET A 221	32.515	18.529	25.517	1.00	21.94
ATOM	1446	N	MET A 222	31.993	16.772	24.253	1.00	25.48
ATOM	1447	CA	MET A 222	33.218	16.013	24.595	1.00	27.01
ATOM	1448	CB	MET A 222	32.953	14.538	24.311	1.00	27.99
ATOM	1449	CG	MET A 222	31.762	14.002	25.081	1.00	29.87
ATOM	1450	SD	MET A 222	32.118	13.649	26.808	1.00	38.44
ATOM	1451	CE	MET A 222	32.621	15.072	27.408	1.00	31.07
ATOM	1452	C	MET A 222	34.518	16.505	23.925	1.00	26.90
ATOM	1453	O	MET A 222	35.593	15.941	24.052	1.00	28.44
ATOM	1454	N	LEU A 223	34.409	17.609	23.222	1.00	27.45
ATOM	1455	CA	LEU A 223	35.564	18.156	22.539	1.00	24.63

Fig. 4CC

ATOM	1456	CB	LEU A 223	35.090	19.049	21.386	1.00	29.39
ATOM	1457	CG	LEU A 223	35.847	19.121	20.049	1.00	24.93
ATOM	1458	CD1	LEU A 223	35.810	17.772	19.381	1.00	23.13
ATOM	1459	CD2	LEU A 223	35.188	20.151	19.127	1.00	28.48
ATOM	1460	C	LEU A 223	36.375	18.937	23.567	1.00	27.48
ATOM	1461	O	LEU A 223	35.886	19.790	24.309	1.00	23.71
ATOM	1462	N	ARG A 224	37.638	18.563	23.667	1.00	34.72
ATOM	1463	CA	ARG A 224	38.562	19.263	24.567	1.00	38.82
ATOM	1464	CB	ARG A 224	39.765	18.382	24.849	1.00	43.75
ATOM	1465	CG	ARG A 224	39.551	17.438	26.006	1.00	55.91
ATOM	1466	CD	ARG A 224	39.000	18.223	27.190	1.00	65.77
ATOM	1467	NE	ARG A 224	39.408	17.708	28.501	1.00	73.29
ATOM	1468	CZ	ARG A 224	39.136	16.489	28.971	1.00	76.88
ATOM	1469	NH1	ARG A 224	39.569	16.154	30.189	1.00	76.89
ATOM	1470	NH2	ARG A 224	38.450	15.605	28.239	1.00	78.31
ATOM	1471	C	ARG A 224	38.965	20.567	23.869	1.00	42.27
ATOM	1472	O	ARG A 224	39.589	20.572	22.800	1.00	44.43
ATOM	1473	N	ASP A 225	38.519	21.677	24.451	1.00	46.11
ATOM	1474	CA	ASP A 225	38.803	23.044	23.902	1.00	49.33
ATOM	1475	CB	ASP A 225	40.225	23.464	24.257	1.00	58.78
ATOM	1476	CG	ASP A 225	40.542	24.890	23.805	1.00	66.98
ATOM	1477	OD1	ASP A 225	40.468	25.809	24.636	1.00	71.51
ATOM	1478	OD2	ASP A 225	40.856	25.114	22.619	1.00	73.88
ATOM	1479	C	ASP A 225	38.614	23.170	22.371	1.00	48.68
ATOM	1480	O	ASP A 225	39.552	23.149	21.620	1.00	51.27
ATOM	1481	N	ARG A 226	37.419	23.413	21.885	1.00	41.79
ATOM	1482	CA	ARG A 226	37.264	23.506	20.421	1.00	33.40
ATOM	1483	CB	ARG A 226	35.786	23.442	20.090	1.00	36.65
ATOM	1484	CG	ARG A 226	35.073	24.708	20.520	1.00	37.55
ATOM	1485	CD	ARG A 226	33.573	24.698	20.287	1.00	37.46
ATOM	1486	NE	ARG A 226	33.120	26.075	20.121	1.00	37.26
ATOM	1487	CZ	ARG A 226	32.833	26.612	18.945	1.00	37.48
ATOM	1488	NH1	ARG A 226	32.461	27.877	18.878	1.00	37.93
ATOM	1489	NH2	ARG A 226	32.857	25.864	17.844	1.00	38.45
ATOM	1490	C	ARG A 226	37.898	24.775	19.805	1.00	29.10
ATOM	1491	O	ARG A 226	38.156	24.849	18.598	1.00	33.55
ATOM	1492	N	TRP A 227	38.094	25.797	20.635	1.00	22.03
ATOM	1493	CA	TRP A 227	38.656	27.091	20.166	1.00	21.39
ATOM	1494	CB	TRP A 227	38.490	28.154	21.249	1.00	22.63
ATOM	1495	CG	TRP A 227	37.077	28.584	21.461	1.00	24.25
ATOM	1496	CD2	TRP A 227	36.249	29.338	20.557	1.00	27.88
ATOM	1497	CE2	TRP A 227	34.975	29.468	21.165	1.00	31.02
ATOM	1498	CE3	TRP A 227	36.458	29.914	19.295	1.00	29.58
ATOM	1499	CD1	TRP A 227	36.297	28.311	22.549	1.00	26.56
ATOM	1500	NE1	TRP A 227	35.036	28.832	22.379	1.00	27.82
ATOM	1501	CZ2	TRP A 227	33.911	30.146	20.552	1.00	28.29
ATOM	1502	CZ3	TRP A 227	35.391	30.598	18.683	1.00	32.75
ATOM	1503	CH2	TRP A 227	34.138	30.703	19.316	1.00	31.24
ATOM	1504	C	TRP A 227	40.113	27.048	19.660	1.00	23.70
ATOM	1505	O	TRP A 227	40.606	27.960	18.977	1.00	27.60
ATOM	1506	N	SER A 228	40.814	25.988	20.040	1.00	18.51
ATOM	1507	CA	SER A 228	42.184	25.798	19.596	1.00	15.81

Fig. 4DD

ATOM	1508	CB	SER A 228	42.815	24.662	20.368	1.00	15.52
ATOM	1509	OG	SER A 228	43.254	25.128	21.616	1.00	17.60
ATOM	1510	C	SER A 228	42.101	25.458	18.119	1.00	14.79
ATOM	1511	O	SER A 228	42.767	26.053	17.266	1.00	21.46
ATOM	1512	N	LEU A 229	41.252	24.477	17.827	1.00	7.62
ATOM	1513	CA	LEU A 229	41.047	24.042	16.448	1.00	7.17
ATOM	1514	CB	LEU A 229	40.018	22.935	16.364	1.00	10.34
ATOM	1515	CG	LEU A 229	40.194	21.741	17.280	1.00	20.72
ATOM	1516	CD1	LEU A 229	39.311	20.598	16.771	1.00	27.16
ATOM	1517	CD2	LEU A 229	41.658	21.326	17.305	1.00	27.96
ATOM	1518	C	LEU A 229	40.585	25.224	15.621	1.00	7.22
ATOM	1519	O	LEU A 229	41.089	25.499	14.537	1.00	8.55
ATOM	1520	N	VAL A 230	39.619	25.959	16.159	1.00	5.89
ATOM	1521	CA	VAL A 230	39.078	27.114	15.432	1.00	5.94
ATOM	1522	CB	VAL A 230	37.922	27.795	16.232	1.00	4.89
ATOM	1523	CG1	VAL A 230	37.419	29.047	15.526	1.00	2.00
ATOM	1524	CG2	VAL A 230	36.773	26.806	16.398	1.00	4.47
ATOM	1525	C	VAL A 230	40.224	28.090	15.072	1.00	6.40
ATOM	1526	O	VAL A 230	40.438	28.506	13.922	1.00	9.66
ATOM	1527	N	ALA A 231	41.052	28.344	16.064	1.00	7.60
ATOM	1528	CA	ALA A 231	42.168	29.268	15.887	1.00	9.93
ATOM	1529	CB	ALA A 231	42.872	29.443	17.201	1.00	8.04
ATOM	1530	C	ALA A 231	43.128	28.732	14.827	1.00	11.60
ATOM	1531	O	ALA A 231	43.551	29.400	13.884	1.00	13.10
ATOM	1532	N	GLU A 232	43.399	27.448	14.957	1.00	10.99
ATOM	1533	CA	GLU A 232	44.305	26.796	14.066	1.00	11.94
ATOM	1534	CB	GLU A 232	44.569	25.399	14.581	1.00	13.60
ATOM	1535	CG	GLU A 232	45.749	24.763	13.928	1.00	29.60
ATOM	1536	CD	GLU A 232	45.731	23.252	14.019	1.00	35.18
ATOM	1537	OE1	GLU A 232	46.359	22.597	13.150	1.00	42.87
ATOM	1538	OE2	GLU A 232	45.085	22.719	14.949	1.00	33.58
ATOM	1539	C	GLU A 232	43.796	26.788	12.623	1.00	13.86
ATOM	1540	O	GLU A 232	44.517	27.157	11.679	1.00	20.91
ATOM	1541	N	ARG A 233	42.522	26.440	12.456	1.00	13.11
ATOM	1542	CA	ARG A 233	41.905	26.342	11.093	1.00	11.31
ATOM	1543	CB	ARG A 233	40.726	25.380	11.138	1.00	12.40
ATOM	1544	CG	ARG A 233	41.091	24.153	11.961	1.00	12.31
ATOM	1545	CD	ARG A 233	40.903	22.852	11.256	1.00	13.86
ATOM	1546	NE	ARG A 233	39.503	22.462	11.296	1.00	16.88
ATOM	1547	CZ	ARG A 233	39.044	21.301	11.764	1.00	19.74
ATOM	1548	NH1	ARG A 233	37.736	21.049	11.757	1.00	17.79
ATOM	1549	NH2	ARG A 233	39.883	20.376	12.213	1.00	18.20
ATOM	1550	C	ARG A 233	41.560	27.694	10.482	1.00	9.84
ATOM	1551	O	ARG A 233	41.376	27.845	9.268	1.00	14.70
ATOM	1552	N	ARG A 234	41.521	28.705	11.339	1.00	9.30
ATOM	1553	CA	ARG A 234	41.297	30.079	10.885	1.00	8.94
ATOM	1554	CB	ARG A 234	41.003	30.993	12.075	1.00	16.51
ATOM	1555	CG	ARG A 234	41.011	32.462	11.684	1.00	25.37
ATOM	1556	CD	ARG A 234	41.146	33.487	12.819	1.00	32.39
ATOM	1557	NE	ARG A 234	41.213	34.830	12.225	1.00	44.51
ATOM	1558	CZ	ARG A 234	40.612	35.934	12.683	1.00	46.54
ATOM	1559	NH1	ARG A 234	39.880	35.913	13.783	1.00	48.43

Fig. 4EE

ATOM	1560	NH2	ARG A 234	40.694	37.064	11.990	1.00	50.93
ATOM	1561	C	ARG A 234	42.615	30.513	10.199	1.00	11.94
ATOM	1562	O	ARG A 234	42.624	31.231	9.196	1.00	14.73
ATOM	1563	N	ARG A 235	43.739	30.106	10.804	1.00	12.37
ATOM	1564	CA	ARG A 235	45.114	30.426	10.286	1.00	16.31
ATOM	1565	CB	ARG A 235	46.170	30.059	11.313	1.00	23.21
ATOM	1566	CG	ARG A 235	46.045	30.880	12.594	1.00	34.61
ATOM	1567	CD	ARG A 235	47.263	30.750	13.491	1.00	37.31
ATOM	1568	NE	ARG A 235	47.521	29.350	13.824	1.00	43.60
ATOM	1569	CZ	ARG A 235	47.264	28.801	15.014	1.00	47.17
ATOM	1570	NH1	ARG A 235	47.535	27.511	15.221	1.00	45.31
ATOM	1571	NH2	ARG A 235	46.748	29.536	16.003	1.00	41.44
ATOM	1572	C	ARG A 235	45.404	29.739	8.969	1.00	15.83
ATOM	1573	O	ARG A 235	45.918	30.328	8.034	1.00	22.48
ATOM	1574	N	GLN A 236	45.058	28.460	8.906	1.00	14.95
ATOM	1575	CA	GLN A 236	45.211	27.650	7.662	1.00	11.72
ATOM	1576	CB	GLN A 236	44.718	26.211	7.886	1.00	11.77
ATOM	1577	CG	GLN A 236	45.357	25.449	9.055	1.00	15.53
ATOM	1578	CD	GLN A 236	44.614	24.163	9.391	1.00	16.00
ATOM	1579	OE1	GLN A 236	43.439	24.006	9.029	1.00	19.46
ATOM	1580	NE2	GLN A 236	45.278	23.252	10.114	1.00	10.57
ATOM	1581	C	GLN A 236	44.436	28.262	6.475	1.00	10.13
ATOM	1582	O	GLN A 236	44.815	28.101	5.324	1.00	15.63
ATOM	1583	N	ALA A 237	43.301	28.898	6.777	1.00	10.03
ATOM	1584	CA	ALA A 237	42.404	29.536	5.742	1.00	9.79
ATOM	1585	CB	ALA A 237	40.972	29.654	6.282	1.00	6.79
ATOM	1586	C	ALA A 237	42.890	30.911	5.264	1.00	10.12
ATOM	1587	O	ALA A 237	42.454	31.444	4.253	1.00	14.25
ATOM	1588	N	GLY A 238	43.813	31.491	6.024	1.00	10.29
ATOM	1589	CA	GLY A 238	44.340	32.789	5.674	1.00	4.75
ATOM	1590	C	GLY A 238	43.355	33.872	6.054	1.00	9.07
ATOM	1591	O	GLY A 238	43.334	34.929	5.424	1.00	8.04
ATOM	1592	N	ILE A 239	42.534	33.604	7.075	1.00	11.44
ATOM	1593	CA	ILE A 239	41.491	34.575	7.555	1.00	11.41
ATOM	1594	CB	ILE A 239	40.310	33.875	8.336	1.00	7.37
ATOM	1595	CG2	ILE A 239	39.322	34.874	8.830	1.00	4.21
ATOM	1596	CG1	ILE A 239	39.544	32.918	7.449	1.00	3.48
ATOM	1597	CD1	ILE A 239	38.562	32.125	8.208	1.00	3.45
ATOM	1598	C	ILE A 239	42.203	35.472	8.527	1.00	13.52
ATOM	1599	O	ILE A 239	42.912	35.017	9.436	1.00	12.69
ATOM	1600	N	ALA A 240	41.991	36.766	8.351	1.00	15.63
ATOM	1601	CA	ALA A 240	42.624	37.747	9.217	1.00	18.89
ATOM	1602	CB	ALA A 240	44.040	38.026	8.729	1.00	25.01
ATOM	1603	C	ALA A 240	41.834	39.029	9.231	1.00	24.53
ATOM	1604	O	ALA A 240	41.179	39.417	8.265	1.00	32.64
ATOM	1605	N	GLY A 241	41.890	39.706	10.363	1.00	26.12
ATOM	1606	CA	GLY A 241	41.196	40.962	10.462	1.00	28.34
ATOM	1607	C	GLY A 241	40.353	41.071	11.700	1.00	28.76
ATOM	1608	O	GLY A 241	40.482	40.318	12.648	1.00	23.53
ATOM	1609	N	HIS A 242	39.489	42.064	11.681	1.00	34.29
ATOM	1610	CA	HIS A 242	38.596	42.332	12.793	1.00	33.42
ATOM	1611	CB	HIS A 242	38.278	43.820	12.786	1.00	38.49

Fig. 4FF

ATOM	1612	CG	HIS A 242	38.080	44.396	14.146	1.00	42.30
ATOM	1613	CD2	HIS A 242	37.279	45.393	14.586	1.00	44.39
ATOM	1614	ND1	HIS A 242	38.763	43.939	15.251	1.00	46.23
ATOM	1615	CE1	HIS A 242	38.389	44.629	16.313	1.00	45.99
ATOM	1616	NE2	HIS A 242	37.489	45.517	15.936	1.00	46.42
ATOM	1617	C	HIS A 242	37.353	41.479	12.565	1.00	31.34
ATOM	1618	O	HIS A 242	36.288	41.957	12.177	1.00	31.77
ATOM	1619	N	THR A 243	37.521	40.182	12.747	1.00	25.13
ATOM	1620	CA	THR A 243	36.401	39.257	12.554	1.00	24.56
ATOM	1621	CB	THR A 243	36.926	37.887	12.060	1.00	27.68
ATOM	1622	OG1	THR A 243	37.816	37.314	13.033	1.00	24.15
ATOM	1623	CG2	THR A 243	37.690	38.064	10.715	1.00	26.23
ATOM	1624	C	THR A 243	35.561	39.124	13.854	1.00	21.74
ATOM	1625	O	THR A 243	35.993	39.525	14.930	1.00	19.85
ATOM	1626	N	TYR A 244	34.313	38.667	13.722	1.00	19.10
ATOM	1627	CA	TYR A 244	33.427	38.457	14.913	1.00	15.57
ATOM	1628	CB	TYR A 244	31.962	38.295	14.532	1.00	14.06
ATOM	1629	CG	TYR A 244	31.306	39.493	13.925	1.00	4.92
ATOM	1630	CD1	TYR A 244	30.688	40.458	14.715	1.00	4.27
ATOM	1631	CE1	TYR A 244	30.045	41.530	14.143	1.00	2.00
ATOM	1632	CD2	TYR A 244	31.261	39.637	12.548	1.00	9.74
ATOM	1633	CE2	TYR A 244	30.623	40.695	11.965	1.00	7.59
ATOM	1634	CZ	TYR A 244	30.015	41.636	12.773	1.00	8.21
ATOM	1635	OH	TYR A 244	29.357	42.669	12.179	1.00	18.77
ATOM	1636	C	TYR A 244	33.862	37.187	15.595	1.00	14.96
ATOM	1637	O	TYR A 244	33.530	36.924	16.738	1.00	19.83
ATOM	1638	N	LEU A 245	34.511	36.329	14.811	1.00	15.53
ATOM	1639	CA	LEU A 245	35.010	35.042	15.318	1.00	16.41
ATOM	1640	CB	LEU A 245	35.716	34.282	14.205	1.00	11.78
ATOM	1641	CG	LEU A 245	36.292	32.945	14.654	1.00	8.82
ATOM	1642	CD1	LEU A 245	35.234	32.102	15.349	1.00	7.84
ATOM	1643	CD2	LEU A 245	36.844	32.242	13.469	1.00	7.03
ATOM	1644	C	LEU A 245	35.954	35.381	16.444	1.00	17.28
ATOM	1645	O	LEU A 245	36.966	36.034	16.252	1.00	24.50
ATOM	1646	N	GLN A 246	35.628	34.889	17.624	1.00	20.92
ATOM	1647	CA	GLN A 246	36.404	35.187	18.855	1.00	25.04
ATOM	1648	CB	GLN A 246	35.435	35.118	20.045	1.00	26.22
ATOM	1649	CG	GLN A 246	35.506	36.290	21.006	1.00	34.07
ATOM	1650	CD	GLN A 246	35.105	37.623	20.379	1.00	38.80
ATOM	1651	OE1	GLN A 246	35.160	37.811	19.166	1.00	33.06
ATOM	1652	NE2	GLN A 246	34.701	38.559	21.222	1.00	45.90
ATOM	1653	C	GLN A 246	37.642	34.285	19.055	1.00	26.29
ATOM	1654	O	GLN A 246	38.038	33.946	20.167	1.00	29.79
ATOM	1655	N	ALA A 247	38.291	33.955	17.949	1.00	28.45
ATOM	1656	CA	ALA A 247	39.452	33.069	17.978	1.00	28.46
ATOM	1657	CB	ALA A 247	38.989	31.631	17.932	1.00	30.30
ATOM	1658	C	ALA A 247	40.328	33.364	16.773	1.00	32.68
ATOM	1659	O	ALA A 247	41.454	32.823	16.705	1.00	38.87
ATOM	1660	OT	ALA A 247	39.871	34.130	15.912	1.00	34.37
ATOM	1661	CB	ALA B 17	7.914	5.748	31.702	1.00	42.04
ATOM	1662	C	ALA B 17	10.186	5.934	32.769	1.00	36.44
ATOM	1663	O	ALA B 17	11.186	5.814	32.063	1.00	36.04

Fig. 4GG

ATOM	1664	N	ALA B	17	8.300	4.683	33.913	1.00	41.59
ATOM	1665	CA	ALA B	17	8.924	5.050	32.589	1.00	39.91
ATOM	1666	N	ALA B	18	10.112	6.843	33.731	1.00	31.29
ATOM	1667	CA	ALA B	18	11.248	7.701	34.016	1.00	27.61
ATOM	1668	CB	ALA B	18	10.834	8.828	34.910	1.00	24.69
ATOM	1669	C	ALA B	18	12.280	6.823	34.725	1.00	29.22
ATOM	1670	O	ALA B	18	11.948	5.839	35.399	1.00	33.49
ATOM	1671	N	VAL B	19	13.546	7.137	34.466	1.00	27.94
ATOM	1672	CA	VAL B	19	14.697	6.453	35.079	1.00	23.42
ATOM	1673	CB	VAL B	19	15.917	6.368	34.124	1.00	21.98
ATOM	1674	CG1	VAL B	19	17.180	6.063	34.899	1.00	22.99
ATOM	1675	CG2	VAL B	19	15.707	5.276	33.094	1.00	22.11
ATOM	1676	C	VAL B	19	15.041	7.441	36.171	1.00	23.75
ATOM	1677	O	VAL B	19	15.320	8.613	35.902	1.00	29.08
ATOM	1678	N	PRO B	20	14.897	7.017	37.439	1.00	24.40
ATOM	1679	CD	PRO B	20	14.336	5.738	37.907	1.00	20.63
ATOM	1680	CA	PRO B	20	15.210	7.897	38.572	1.00	16.99
ATOM	1681	CB	PRO B	20	14.681	7.118	39.773	1.00	17.30
ATOM	1682	CG	PRO B	20	13.659	6.171	39.176	1.00	22.30
ATOM	1683	C	PRO B	20	16.735	8.039	38.627	1.00	15.71
ATOM	1684	O	PRO B	20	17.501	7.083	38.650	1.00	21.58
ATOM	1685	N	ILE B	21	17.186	9.266	38.594	1.00	12.31
ATOM	1686	CA	ILE B	21	18.595	9.500	38.613	1.00	10.03
ATOM	1687	CB	ILE B	21	18.979	10.413	37.430	1.00	11.03
ATOM	1688	CG2	ILE B	21	20.393	10.889	37.540	1.00	13.92
ATOM	1689	CG1	ILE B	21	18.828	9.672	36.106	1.00	9.00
ATOM	1690	CD1	ILE B	21	18.934	10.589	34.911	1.00	7.24
ATOM	1691	C	ILE B	21	18.867	10.215	39.901	1.00	13.47
ATOM	1692	O	ILE B	21	18.120	11.101	40.315	1.00	19.72
ATOM	1693	N	TYR B	22	19.933	9.791	40.567	1.00	14.67
ATOM	1694	CA	TYR B	22	20.410	10.416	41.827	1.00	13.36
ATOM	1695	CB	TYR B	22	20.804	9.351	42.841	1.00	14.24
ATOM	1696	CG	TYR B	22	19.639	8.560	43.295	1.00	14.90
ATOM	1697	CD1	TYR B	22	18.899	8.958	44.407	1.00	19.97
ATOM	1698	CE1	TYR B	22	17.735	8.300	44.763	1.00	21.18
ATOM	1699	CD2	TYR B	22	19.203	7.482	42.564	1.00	13.21
ATOM	1700	CE2	TYR B	22	18.053	6.818	42.909	1.00	19.45
ATOM	1701	CZ	TYR B	22	17.317	7.231	44.003	1.00	19.77
ATOM	1702	OH	TYR B	22	16.148	6.579	44.303	1.00	24.12
ATOM	1703	C	TYR B	22	21.628	11.324	41.562	1.00	12.70
ATOM	1704	O	TYR B	22	22.625	10.918	40.965	1.00	9.15
ATOM	1705	N	VAL B	23	21.531	12.557	42.040	1.00	14.63
ATOM	1706	CA	VAL B	23	22.629	13.540	41.904	1.00	16.43
ATOM	1707	CB	VAL B	23	22.123	14.954	41.556	1.00	17.71
ATOM	1708	CG1	VAL B	23	23.072	15.636	40.554	1.00	15.98
ATOM	1709	CG2	VAL B	23	20.685	14.909	41.081	1.00	17.96
ATOM	1710	C	VAL B	23	23.207	13.671	43.305	1.00	16.17
ATOM	1711	O	VAL B	23	22.493	13.693	44.302	1.00	18.84
ATOM	1712	N	ALA B	24	24.511	13.850	43.374	1.00	15.31
ATOM	1713	CA	ALA B	24	25.196	14.016	44.676	1.00	14.89
ATOM	1714	CB	ALA B	24	25.689	12.667	45.201	1.00	12.44
ATOM	1715	C	ALA B	24	26.381	14.936	44.414	1.00	14.63

Fig. 4HH

ATOM	1716	O	ALA B	24	26.930	14.969	43.308	1.00	15.05
ATOM	1717	N	GLY B	25	26.729	15.731	45.423	1.00	12.31
ATOM	1718	CA	GLY B	25	27.860	16.623	45.310	1.00	5.61
ATOM	1719	C	GLY B	25	27.865	17.640	46.411	1.00	5.51
ATOM	1720	O	GLY B	25	27.029	17.585	47.284	1.00	12.72
ATOM	1721	N	PHE B	26	28.854	18.518	46.416	1.00	6.35
ATOM	1722	CA	PHE B	26	28.940	19.590	47.405	1.00	7.67
ATOM	1723	CB	PHE B	26	30.389	19.864	47.792	1.00	9.57
ATOM	1724	CG	PHE B	26	30.949	18.878	48.767	1.00	13.16
ATOM	1725	CD1	PHE B	26	31.679	17.773	48.328	1.00	11.14
ATOM	1726	CD2	PHE B	26	30.731	19.039	50.134	1.00	11.34
ATOM	1727	CE1	PHE B	26	32.184	16.834	49.253	1.00	13.74
ATOM	1728	CE2	PHE B	26	31.230	18.110	51.061	1.00	7.30
ATOM	1729	CZ	PHE B	26	31.953	17.011	50.627	1.00	7.04
ATOM	1730	C	PHE B	26	28.298	20.843	46.770	1.00	9.17
ATOM	1731	O	PHE B	26	28.474	21.176	45.581	1.00	11.18
ATOM	1732	N	LEU B	27	27.440	21.467	47.559	1.00	5.05
ATOM	1733	CA	LEU B	27	26.750	22.682	47.145	1.00	4.57
ATOM	1734	CB	LEU B	27	25.548	22.902	48.065	1.00	8.98
ATOM	1735	CG	LEU B	27	24.093	22.598	47.642	1.00	9.54
ATOM	1736	CD1	LEU B	27	24.012	22.036	46.225	1.00	8.26
ATOM	1737	CD2	LEU B	27	23.453	21.669	48.614	1.00	3.57
ATOM	1738	C	LEU B	27	27.788	23.805	47.279	1.00	6.30
ATOM	1739	O	LEU B	27	27.705	24.847	46.651	1.00	9.86
ATOM	1740	N	ALA B	28	28.800	23.539	48.097	1.00	5.73
ATOM	1741	CA	ALA B	28	29.898	24.487	48.379	1.00	7.39
ATOM	1742	CB	ALA B	28	29.332	25.732	49.016	1.00	4.11
ATOM	1743	C	ALA B	28	30.983	23.851	49.319	1.00	12.09
ATOM	1744	O	ALA B	28	30.745	22.923	50.101	1.00	10.48
ATOM	1745	N	LEU B	29	32.218	24.297	49.141	1.00	15.20
ATOM	1746	CA	LEU B	29	33.331	23.837	49.999	1.00	17.93
ATOM	1747	CB	LEU B	29	34.550	23.538	49.145	1.00	17.09
ATOM	1748	CG	LEU B	29	34.431	22.363	48.194	1.00	12.85
ATOM	1749	CD1	LEU B	29	35.778	22.222	47.469	1.00	13.89
ATOM	1750	CD2	LEU B	29	34.087	21.108	48.956	1.00	7.88
ATOM	1751	C	LEU B	29	33.600	25.025	50.968	1.00	18.65
ATOM	1752	O	LEU B	29	33.623	26.197	50.554	1.00	20.18
ATOM	1753	N	TYR B	30	33.810	24.706	52.248	1.00	18.71
ATOM	1754	CA	TYR B	30	34.028	25.738	53.309	1.00	19.45
ATOM	1755	CB	TYR B	30	33.951	25.113	54.704	1.00	15.67
ATOM	1756	CG	TYR B	30	32.538	24.795	55.139	1.00	13.40
ATOM	1757	CD1	TYR B	30	31.514	25.724	54.983	1.00	8.00
ATOM	1758	CE1	TYR B	30	30.213	25.422	55.378	1.00	8.39
ATOM	1759	CD2	TYR B	30	32.223	23.554	55.700	1.00	15.68
ATOM	1760	CE2	TYR B	30	30.912	23.241	56.104	1.00	7.37
ATOM	1761	CZ	TYR B	30	29.925	24.184	55.938	1.00	5.65
ATOM	1762	OH	TYR B	30	28.657	23.910	56.351	1.00	8.42
ATOM	1763	C	TYR B	30	35.233	26.657	53.213	1.00	23.64
ATOM	1764	O	TYR B	30	35.094	27.881	53.294	1.00	31.45
ATOM	1765	N	ASP B	31	36.432	26.100	53.067	1.00	23.40
ATOM	1766	CA	ASP B	31	37.626	26.995	52.963	1.00	28.47
ATOM	1767	CB	ASP B	31	38.533	26.833	54.207	1.00	37.77

Fig. 4II

ATOM	1768	CG	ASP	B	31	38.070	27.693	55.427	1.00	43.27
ATOM	1769	OD1	ASP	B	31	37.920	27.126	56.541	1.00	46.07
ATOM	1770	OD2	ASP	B	31	37.900	28.933	55.286	1.00	41.65
ATOM	1771	C	ASP	B	31	38.386	26.745	51.641	1.00	27.15
ATOM	1772	O	ASP	B	31	39.570	26.399	51.588	1.00	30.69
ATOM	1773	N	SER	B	32	37.680	27.020	50.555	1.00	24.54
ATOM	1774	CA	SER	B	32	38.202	26.778	49.219	1.00	20.41
ATOM	1775	CB	SER	B	32	37.112	26.114	48.387	1.00	21.75
ATOM	1776	OG	SER	B	32	35.933	26.899	48.408	1.00	26.20
ATOM	1777	C	SER	B	32	38.758	27.974	48.497	1.00	20.84
ATOM	1778	O	SER	B	32	39.635	27.855	47.661	1.00	23.98
ATOM	1779	N	GLY	B	33	38.226	29.146	48.785	1.00	20.77
ATOM	1780	CA	GLY	B	33	38.705	30.318	48.081	1.00	16.03
ATOM	1781	C	GLY	B	33	37.617	30.952	47.236	1.00	19.69
ATOM	1782	O	GLY	B	33	37.920	31.559	46.217	1.00	19.90
ATOM	1783	N	ASP	B	34	36.351	30.791	47.642	1.00	22.84
ATOM	1784	CA	ASP	B	34	35.194	31.407	46.915	1.00	23.86
ATOM	1785	CB	ASP	B	34	33.849	30.858	47.437	1.00	20.39
ATOM	1786	CG	ASP	B	34	33.467	29.505	46.845	1.00	20.19
ATOM	1787	OD1	ASP	B	34	32.923	28.659	47.594	1.00	19.43
ATOM	1788	OD2	ASP	B	34	33.655	29.287	45.636	1.00	21.35
ATOM	1789	C	ASP	B	34	35.262	32.941	47.180	1.00	28.22
ATOM	1790	O	ASP	B	34	35.542	33.385	48.295	1.00	29.13
ATOM	1791	N	PRO	B	35	35.030	33.765	46.141	1.00	29.64
ATOM	1792	CD	PRO	B	35	34.740	33.415	44.737	1.00	34.16
ATOM	1793	CA	PRO	B	35	35.066	35.217	46.319	1.00	30.50
ATOM	1794	CB	PRO	B	35	34.454	35.724	45.021	1.00	33.09
ATOM	1795	CG	PRO	B	35	34.952	34.726	44.024	1.00	33.02
ATOM	1796	C	PRO	B	35	34.205	35.636	47.522	1.00	32.77
ATOM	1797	O	PRO	B	35	33.386	34.867	48.044	1.00	34.58
ATOM	1798	N	GLY	B	36	34.344	36.902	47.903	1.00	33.77
ATOM	1799	CA	GLY	B	36	33.596	37.424	49.035	1.00	35.99
ATOM	1800	C	GLY	B	36	32.138	37.010	49.117	1.00	36.20
ATOM	1801	O	GLY	B	36	31.723	36.316	50.042	1.00	35.68
ATOM	1802	N	GLU	B	37	31.369	37.434	48.126	1.00	37.95
ATOM	1803	CA	GLU	B	37	29.933	37.137	48.051	1.00	37.96
ATOM	1804	CB	GLU	B	37	29.401	37.840	46.796	1.00	45.40
ATOM	1805	CG	GLU	B	37	27.957	37.539	46.417	1.00	58.85
ATOM	1806	CD	GLU	B	37	27.524	38.252	45.126	1.00	65.53
ATOM	1807	OE1	GLU	B	37	28.214	38.093	44.086	1.00	66.48
ATOM	1808	OE2	GLU	B	37	26.494	38.977	45.156	1.00	69.68
ATOM	1809	C	GLU	B	37	29.537	35.621	48.101	1.00	35.52
ATOM	1810	O	GLU	B	37	28.801	35.172	48.976	1.00	40.65
ATOM	1811	N	LEU	B	38	30.091	34.821	47.198	1.00	28.34
ATOM	1812	CA	LEU	B	38	29.715	33.384	47.117	1.00	20.64
ATOM	1813	CB	LEU	B	38	30.289	32.807	45.842	1.00	19.87
ATOM	1814	CG	LEU	B	38	29.891	33.584	44.600	1.00	19.38
ATOM	1815	CD1	LEU	B	38	30.515	32.915	43.399	1.00	21.32
ATOM	1816	CD2	LEU	B	38	28.374	33.625	44.484	1.00	20.57
ATOM	1817	C	LEU	B	38	30.056	32.479	48.285	1.00	19.55
ATOM	1818	O	LEU	B	38	29.484	31.410	48.494	1.00	16.14
ATOM	1819	N	ALA	B	39	31.042	32.914	49.043	1.00	21.73

Fig. 4JJ

ATOM	1820	CA	ALA B	39	31.535	32.138	50.189	1.00	23.75
ATOM	1821	CB	ALA B	39	32.594	32.925	50.916	1.00	23.17
ATOM	1822	C	ALA B	39	30.470	31.681	51.173	1.00	22.95
ATOM	1823	O	ALA B	39	29.624	32.445	51.621	1.00	30.93
ATOM	1824	N	LEU B	40	30.565	30.412	51.543	1.00	21.62
ATOM	1825	CA	LEU B	40	29.645	29.799	52.517	1.00	23.96
ATOM	1826	CB	LEU B	40	28.877	28.665	51.836	1.00	24.40
ATOM	1827	CG	LEU B	40	27.534	29.021	51.176	1.00	26.75
ATOM	1828	CD1	LEU B	40	26.934	27.779	50.575	1.00	24.00
ATOM	1829	CD2	LEU B	40	26.533	29.598	52.192	1.00	25.11
ATOM	1830	C	LEU B	40	30.436	29.293	53.757	1.00	23.95
ATOM	1831	O	LEU B	40	31.531	28.783	53.634	1.00	27.29
ATOM	1832	N	ASP B	41	29.892	29.461	54.960	1.00	24.27
ATOM	1833	CA	ASP B	41	30.598	28.978	56.171	1.00	20.70
ATOM	1834	CB	ASP B	41	31.074	30.151	56.983	1.00	24.18
ATOM	1835	CG	ASP B	41	29.959	31.045	57.375	1.00	28.70
ATOM	1836	OD1	ASP B	41	29.490	30.924	58.524	1.00	35.82
ATOM	1837	OD2	ASP B	41	29.542	31.857	56.522	1.00	38.93
ATOM	1838	C	ASP B	41	29.698	28.043	56.993	1.00	22.49
ATOM	1839	O	ASP B	41	28.474	28.092	56.891	1.00	23.03
ATOM	1840	N	PRO B	42	30.309	27.223	57.884	1.00	22.42
ATOM	1841	CD	PRO B	42	31.738	27.246	58.252	1.00	17.94
ATOM	1842	CA	PRO B	42	29.605	26.256	58.729	1.00	18.37
ATOM	1843	CB	PRO B	42	30.709	25.733	59.644	1.00	17.62
ATOM	1844	CG	PRO B	42	31.930	25.875	58.836	1.00	12.63
ATOM	1845	C	PRO B	42	28.448	26.783	59.529	1.00	20.50
ATOM	1846	O	PRO B	42	27.405	26.160	59.612	1.00	26.91
ATOM	1847	N	ASP B	43	28.613	27.952	60.125	1.00	22.41
ATOM	1848	CA	ASP B	43	27.514	28.502	60.949	1.00	27.41
ATOM	1849	CB	ASP B	43	28.013	29.678	61.782	1.00	29.40
ATOM	1850	CG	ASP B	43	28.516	29.236	63.138	1.00	35.28
ATOM	1851	OD1	ASP B	43	27.886	28.323	63.733	1.00	37.31
ATOM	1852	OD2	ASP B	43	29.535	29.800	63.603	1.00	41.37
ATOM	1853	C	ASP B	43	26.257	28.857	60.148	1.00	27.94
ATOM	1854	O	ASP B	43	25.133	28.474	60.492	1.00	28.82
ATOM	1855	N	THR B	44	26.469	29.558	59.038	1.00	26.47
ATOM	1856	CA	THR B	44	25.357	29.936	58.151	1.00	24.65
ATOM	1857	CB	THR B	44	25.863	30.714	56.935	1.00	27.18
ATOM	1858	OG1	THR B	44	26.592	31.867	57.374	1.00	33.19
ATOM	1859	CG2	THR B	44	24.699	31.168	56.084	1.00	29.04
ATOM	1860	C	THR B	44	24.629	28.672	57.637	1.00	23.56
ATOM	1861	O	THR B	44	23.412	28.632	57.505	1.00	26.17
ATOM	1862	N	VAL B	45	25.397	27.632	57.342	1.00	18.56
ATOM	1863	CA	VAL B	45	24.805	26.391	56.835	1.00	19.89
ATOM	1864	CB	VAL B	45	25.882	25.472	56.271	1.00	21.82
ATOM	1865	CG1	VAL B	45	25.289	24.119	55.829	1.00	18.35
ATOM	1866	CG2	VAL B	45	26.575	26.185	55.120	1.00	18.96
ATOM	1867	C	VAL B	45	24.044	25.702	57.948	1.00	22.56
ATOM	1868	O	VAL B	45	22.943	25.166	57.756	1.00	22.28
ATOM	1869	N	ARG B	46	24.634	25.768	59.140	1.00	24.52
ATOM	1870	CA	ARG B	46	24.037	25.160	60.355	1.00	25.74
ATOM	1871	CB	ARG B	46	24.914	25.485	61.587	1.00	29.95

Fig. 4KK

ATOM	1872	CG	ARG B	46	24.762	24.524	62.809	1.00	39.07
ATOM	1873	CD	ARG B	46	25.326	23.065	62.570	1.00	50.64
ATOM	1874	NE	ARG B	46	24.547	22.250	61.617	1.00	57.51
ATOM	1875	CZ	ARG B	46	24.746	20.952	61.373	1.00	56.52
ATOM	1876	NH1	ARG B	46	23.981	20.315	60.480	1.00	56.75
ATOM	1877	NH2	ARG B	46	25.686	20.282	62.032	1.00	55.99
ATOM	1878	C	ARG B	46	22.598	25.720	60.515	1.00	24.14
ATOM	1879	O	ARG B	46	21.592	25.009	60.593	1.00	27.14
ATOM	1880	N	ALA B	47	22.531	27.037	60.466	1.00	17.85
ATOM	1881	CA	ALA B	47	21.270	27.766	60.603	1.00	19.04
ATOM	1882	CB	ALA B	47	21.551	29.253	60.647	1.00	18.30
ATOM	1883	C	ALA B	47	20.262	27.496	59.501	1.00	19.75
ATOM	1884	O	ALA B	47	19.072	27.650	59.701	1.00	26.03
ATOM	1885	N	ALA B	48	20.745	27.149	58.313	1.00	23.65
ATOM	1886	CA	ALA B	48	19.865	26.905	57.132	1.00	20.82
ATOM	1887	CB	ALA B	48	20.610	27.271	55.877	1.00	17.62
ATOM	1888	C	ALA B	48	19.301	25.473	57.005	1.00	23.83
ATOM	1889	O	ALA B	48	18.437	25.184	56.167	1.00	26.26
ATOM	1890	N	LEU B	49	19.777	24.575	57.859	1.00	24.28
ATOM	1891	CA	LEU B	49	19.336	23.172	57.792	1.00	25.26
ATOM	1892	CB	LEU B	49	20.565	22.268	57.684	1.00	24.55
ATOM	1893	CG	LEU B	49	21.621	22.694	56.663	1.00	23.31
ATOM	1894	CD1	LEU B	49	22.852	21.816	56.752	1.00	21.74
ATOM	1895	CD2	LEU B	49	21.031	22.660	55.276	1.00	19.41
ATOM	1896	C	LEU B	49	18.494	22.796	59.005	1.00	27.28
ATOM	1897	O	LEU B	49	18.781	23.232	60.115	1.00	28.03
ATOM	1898	N	PRO B	50	17.378	22.051	58.789	1.00	29.74
ATOM	1899	CD	PRO B	50	16.528	21.489	59.855	1.00	30.25
ATOM	1900	CA	PRO B	50	16.912	21.585	57.476	1.00	27.96
ATOM	1901	CB	PRO B	50	15.817	20.566	57.826	1.00	24.32
ATOM	1902	CG	PRO B	50	16.089	20.190	59.252	1.00	28.79
ATOM	1903	C	PRO B	50	16.287	22.775	56.731	1.00	25.57
ATOM	1904	O	PRO B	50	15.964	23.810	57.311	1.00	22.54
ATOM	1905	N	PRO B	51	16.157	22.650	55.405	1.00	29.98
ATOM	1906	CD	PRO B	51	16.621	21.587	54.490	1.00	30.02
ATOM	1907	CA	PRO B	51	15.560	23.759	54.659	1.00	30.08
ATOM	1908	CB	PRO B	51	15.657	23.284	53.207	1.00	29.23
ATOM	1909	CG	PRO B	51	16.826	22.344	53.217	1.00	27.99
ATOM	1910	C	PRO B	51	14.090	23.883	55.103	1.00	28.49
ATOM	1911	O	PRO B	51	13.410	22.890	55.392	1.00	24.66
ATOM	1912	N	GLU B	52	13.628	25.128	55.189	1.00	30.06
ATOM	1913	CA	GLU B	52	12.234	25.421	55.589	1.00	32.42
ATOM	1914	CB	GLU B	52	11.956	26.919	55.534	1.00	36.65
ATOM	1915	CG	GLU B	52	10.534	27.287	55.969	1.00	45.10
ATOM	1916	CD	GLU B	52	10.232	26.921	57.426	1.00	48.70
ATOM	1917	OE1	GLU B	52	9.896	25.738	57.705	1.00	48.23
ATOM	1918	OE2	GLU B	52	10.330	27.827	58.293	1.00	51.11
ATOM	1919	C	GLU B	52	11.325	24.679	54.636	1.00	31.01
ATOM	1920	O	GLU B	52	10.443	23.924	55.025	1.00	32.65
ATOM	1921	N	ASN B	53	11.592	24.884	53.352	1.00	33.12
ATOM	1922	CA	ASN B	53	10.824	24.222	52.280	1.00	34.05
ATOM	1923	CB	ASN B	53	10.056	25.273	51.489	1.00	40.45

Fig. 4LL

ATOM	1924	CG	ASN B	53	8.798	25.729	52.212	1.00	47.92
ATOM	1925	OD1	ASN B	53	8.737	26.855	52.716	1.00	51.57
ATOM	1926	ND2	ASN B	53	7.787	24.846	52.283	1.00	47.09
ATOM	1927	C	ASN B	53	11.734	23.363	51.374	1.00	30.06
ATOM	1928	O	ASN B	53	12.924	23.616	51.226	1.00	29.95
ATOM	1929	N	PRO B	54	11.175	22.287	50.800	1.00	27.48
ATOM	1930	CD	PRO B	54	9.757	21.907	50.877	1.00	29.87
ATOM	1931	CA	PRO B	54	11.899	21.371	49.912	1.00	24.96
ATOM	1932	CB	PRO B	54	10.774	20.588	49.244	1.00	26.24
ATOM	1933	CG	PRO B	54	9.770	20.509	50.300	1.00	29.13
ATOM	1934	C	PRO B	54	12.653	22.158	48.861	1.00	20.54
ATOM	1935	O	PRO B	54	12.241	23.235	48.437	1.00	21.35
ATOM	1936	N	LEU B	55	13.779	21.615	48.436	1.00	19.79
ATOM	1937	CA	LEU B	55	14.563	22.315	47.407	1.00	17.15
ATOM	1938	CB	LEU B	55	16.064	22.350	47.781	1.00	18.83
ATOM	1939	CG	LEU B	55	16.558	23.207	48.963	1.00	14.00
ATOM	1940	CD1	LEU B	55	18.025	23.029	49.110	1.00	15.20
ATOM	1941	CD2	LEU B	55	16.277	24.667	48.746	1.00	12.68
ATOM	1942	C	LEU B	55	14.299	21.641	46.046	1.00	12.16
ATOM	1943	O	LEU B	55	14.511	20.442	45.838	1.00	15.08
ATOM	1944	N	PRO B	56	13.675	22.390	45.142	1.00	7.04
ATOM	1945	CD	PRO B	56	13.127	23.752	45.196	1.00	3.73
ATOM	1946	CA	PRO B	56	13.426	21.767	43.853	1.00	10.23
ATOM	1947	CB	PRO B	56	12.415	22.725	43.232	1.00	7.30
ATOM	1948	CG	PRO B	56	12.859	24.046	43.760	1.00	5.82
ATOM	1949	C	PRO B	56	14.771	21.812	43.090	1.00	11.89
ATOM	1950	O	PRO B	56	15.706	22.550	43.446	1.00	8.62
ATOM	1951	N	ILE B	57	14.898	20.968	42.077	1.00	13.53
ATOM	1952	CA	ILE B	57	16.125	20.996	41.238	1.00	9.97
ATOM	1953	CB	ILE B	57	16.791	19.630	41.091	1.00	5.65
ATOM	1954	CG2	ILE B	57	18.004	19.778	40.192	1.00	9.75
ATOM	1955	CG1	ILE B	57	17.274	19.121	42.441	1.00	4.70
ATOM	1956	CD1	ILE B	57	17.866	17.721	42.389	1.00	5.11
ATOM	1957	C	ILE B	57	15.677	21.426	39.845	1.00	9.36
ATOM	1958	O	ILE B	57	14.664	20.937	39.316	1.00	10.17
ATOM	1959	N	ASN B	58	16.349	22.422	39.285	1.00	9.18
ATOM	1960	CA	ASN B	58	15.979	22.813	37.919	1.00	9.79
ATOM	1961	CB	ASN B	58	15.138	24.098	37.883	1.00	15.10
ATOM	1962	CG	ASN B	58	15.657	25.182	38.786	1.00	21.46
ATOM	1963	OD1	ASN B	58	16.813	25.558	38.711	1.00	27.70
ATOM	1964	ND2	ASN B	58	14.773	25.741	39.611	1.00	23.05
ATOM	1965	C	ASN B	58	17.193	22.882	37.029	1.00	7.41
ATOM	1966	O	ASN B	58	18.297	22.619	37.452	1.00	8.49
ATOM	1967	N	VAL B	59	16.965	23.052	35.738	1.00	10.81
ATOM	1968	CA	VAL B	59	18.081	23.178	34.788	1.00	8.30
ATOM	1969	CB	VAL B	59	17.776	22.591	33.427	1.00	6.35
ATOM	1970	CG1	VAL B	59	18.923	22.844	32.503	1.00	9.43
ATOM	1971	CG2	VAL B	59	17.543	21.118	33.532	1.00	11.08
ATOM	1972	C	VAL B	59	18.377	24.662	34.586	1.00	14.22
ATOM	1973	O	VAL B	59	17.490	25.489	34.378	1.00	14.62
ATOM	1974	N	ASP B	60	19.653	24.994	34.744	1.00	22.05
ATOM	1975	CA	ASP B	60	20.173	26.361	34.544	1.00	29.65

Fig. 4MM

ATOM	1976	CB	ASP	B	60	20.522	26.502	33.054	1.00	36.44
ATOM	1977	CG	ASP	B	60	21.635	27.489	32.796	1.00	39.69
ATOM	1978	OD1	ASP	B	60	22.698	27.401	33.449	1.00	42.99
ATOM	1979	OD2	ASP	B	60	21.446	28.343	31.910	1.00	45.07
ATOM	1980	C	ASP	B	60	19.253	27.517	35.047	1.00	33.50
ATOM	1981	O	ASP	B	60	18.875	28.427	34.309	1.00	38.95
ATOM	1982	N	HIS	B	61	18.884	27.447	36.321	1.00	34.75
ATOM	1983	CA	HIS	B	61	18.051	28.492	36.991	1.00	42.36
ATOM	1984	CB	HIS	B	61	18.920	29.705	37.300	1.00	43.73
ATOM	1985	CG	HIS	B	61	19.841	29.482	38.452	1.00	50.34
ATOM	1986	CD2	HIS	B	61	19.579	29.236	39.759	1.00	54.56
ATOM	1987	ND1	HIS	B	61	21.210	29.409	38.317	1.00	51.49
ATOM	1988	CE1	HIS	B	61	21.751	29.123	39.485	1.00	56.03
ATOM	1989	NE2	HIS	B	61	20.784	29.014	40.379	1.00	56.93
ATOM	1990	C	HIS	B	61	16.709	28.940	36.390	1.00	46.16
ATOM	1991	O	HIS	B	61	15.989	29.790	36.949	1.00	46.73
ATOM	1992	N	ARG	B	62	16.393	28.373	35.229	1.00	48.44
ATOM	1993	CA	ARG	B	62	15.128	28.648	34.535	1.00	44.01
ATOM	1994	CB	ARG	B	62	15.220	28.078	33.142	1.00	49.05
ATOM	1995	CG	ARG	B	62	15.701	29.073	32.106	1.00	57.87
ATOM	1996	CD	ARG	B	62	14.543	30.004	31.734	1.00	65.09
ATOM	1997	NE	ARG	B	62	13.269	29.280	31.569	1.00	70.00
ATOM	1998	CZ	ARG	B	62	12.725	28.929	30.399	1.00	70.84
ATOM	1999	NH1	ARG	B	62	13.323	29.232	29.248	1.00	73.75
ATOM	2000	NH2	ARG	B	62	11.585	28.242	30.382	1.00	68.33
ATOM	2001	C	ARG	B	62	14.136	27.892	35.393	1.00	41.14
ATOM	2002	O	ARG	B	62	13.952	26.685	35.287	1.00	40.32
ATOM	2003	N	ALA	B	63	13.562	28.617	36.341	1.00	40.60
ATOM	2004	CA	ALA	B	63	12.598	28.026	37.299	1.00	37.84
ATOM	2005	CB	ALA	B	63	12.014	29.100	38.173	1.00	42.36
ATOM	2006	C	ALA	B	63	11.482	27.183	36.672	1.00	36.34
ATOM	2007	O	ALA	B	63	10.871	26.351	37.319	1.00	33.91
ATOM	2008	N	ARG	B	64	11.210	27.412	35.395	1.00	36.32
ATOM	2009	CA	ARG	B	64	10.171	26.624	34.711	1.00	37.08
ATOM	2010	CB	ARG	B	64	9.886	27.184	33.320	1.00	42.01
ATOM	2011	CG	ARG	B	64	9.199	28.527	33.337	1.00	54.78
ATOM	2012	CD	ARG	B	64	8.008	28.554	32.373	1.00	65.40
ATOM	2013	NE	ARG	B	64	7.263	29.806	32.507	1.00	75.40
ATOM	2014	CZ	ARG	B	64	7.000	30.689	31.539	1.00	76.53
ATOM	2015	NH1	ARG	B	64	6.325	31.784	31.862	1.00	76.03
ATOM	2016	NH2	ARG	B	64	7.366	30.498	30.273	1.00	77.64
ATOM	2017	C	ARG	B	64	10.574	25.157	34.602	1.00	33.67
ATOM	2018	O	ARG	B	64	9.753	24.243	34.608	1.00	37.87
ATOM	2019	N	CYS	B	65	11.876	24.933	34.536	1.00	29.33
ATOM	2020	CA	CYS	B	65	12.396	23.568	34.369	1.00	24.28
ATOM	2021	CB	CYS	B	65	13.633	23.582	33.511	1.00	21.75
ATOM	2022	SG	CYS	B	65	13.207	23.996	31.891	1.00	23.63
ATOM	2023	C	CYS	B	65	12.654	22.743	35.579	1.00	22.51
ATOM	2024	O	CYS	B	65	13.744	22.204	35.784	1.00	24.06
ATOM	2025	N	GLU	B	66	11.628	22.597	36.392	1.00	17.47
ATOM	2026	CA	GLU	B	66	11.791	21.768	37.557	1.00	12.75
ATOM	2027	CB	GLU	B	66	10.643	21.994	38.503	1.00	17.98

Fig. 4NN

ATOM	2028	CG	GLU	B	66	10.845	21.307	39.819	1.00	21.40
ATOM	2029	CD	GLU	B	66	9.909	21.803	40.883	1.00	16.46
ATOM	2030	OE1	GLU	B	66	9.787	23.031	41.030	1.00	19.74
ATOM	2031	OE2	GLU	B	66	9.331	20.957	41.588	1.00	21.07
ATOM	2032	C	GLU	B	66	11.814	20.338	37.006	1.00	12.59
ATOM	2033	O	GLU	B	66	10.920	19.923	36.259	1.00	11.32
ATOM	2034	N	VAL	B	67	12.888	19.616	37.338	1.00	8.95
ATOM	2035	CA	VAL	B	67	13.083	18.216	36.883	1.00	3.32
ATOM	2036	CB	VAL	B	67	14.267	18.100	35.885	1.00	8.56
ATOM	2037	CG1	VAL	B	67	14.033	18.951	34.635	1.00	2.00
ATOM	2038	CG2	VAL	B	67	15.561	18.506	36.565	1.00	2.00
ATOM	2039	C	VAL	B	67	13.364	17.251	38.063	1.00	4.22
ATOM	2040	O	VAL	B	67	13.470	16.032	37.898	1.00	5.26
ATOM	2041	N	GLY	B	68	13.513	17.795	39.263	1.00	2.00
ATOM	2042	CA	GLY	B	68	13.758	16.937	40.403	1.00	2.00
ATOM	2043	C	GLY	B	68	13.611	17.600	41.760	1.00	4.97
ATOM	2044	O	GLY	B	68	13.186	18.759	41.886	1.00	6.51
ATOM	2045	N	ARG	B	69	14.023	16.874	42.789	1.00	5.96
ATOM	2046	CA	ARG	B	69	13.901	17.365	44.160	1.00	11.64
ATOM	2047	CB	ARG	B	69	12.568	16.892	44.746	1.00	12.82
ATOM	2048	CG	ARG	B	69	12.335	17.260	46.204	1.00	16.69
ATOM	2049	CD	ARG	B	69	12.028	18.729	46.379	1.00	19.84
ATOM	2050	NE	ARG	B	69	10.802	19.122	45.698	1.00	22.42
ATOM	2051	CZ	ARG	B	69	9.602	18.674	46.039	1.00	25.63
ATOM	2052	NH1	ARG	B	69	8.530	19.094	45.380	1.00	28.55
ATOM	2053	NH2	ARG	B	69	9.474	17.787	47.019	1.00	19.16
ATOM	2054	C	ARG	B	69	15.056	16.876	45.014	1.00	13.29
ATOM	2055	O	ARG	B	69	15.429	15.702	44.987	1.00	13.90
ATOM	2056	N	VAL	B	70	15.633	17.833	45.740	1.00	12.54
ATOM	2057	CA	VAL	B	70	16.750	17.628	46.705	1.00	12.50
ATOM	2058	CB	VAL	B	70	17.296	18.999	47.162	1.00	7.84
ATOM	2059	CG1	VAL	B	70	18.149	18.854	48.367	1.00	5.53
ATOM	2060	CG2	VAL	B	70	18.058	19.662	46.021	1.00	9.22
ATOM	2061	C	VAL	B	70	16.178	16.867	47.951	1.00	14.23
ATOM	2062	O	VAL	B	70	15.295	17.340	48.668	1.00	16.82
ATOM	2063	N	LEU	B	71	16.701	15.668	48.172	1.00	14.05
ATOM	2064	CA	LEU	B	71	16.258	14.788	49.279	1.00	12.96
ATOM	2065	CB	LEU	B	71	16.509	13.340	48.896	1.00	11.47
ATOM	2066	CG	LEU	B	71	15.921	12.871	47.565	1.00	17.63
ATOM	2067	CD1	LEU	B	71	16.274	11.394	47.305	1.00	19.17
ATOM	2068	CD2	LEU	B	71	14.426	13.049	47.573	1.00	19.25
ATOM	2069	C	LEU	B	71	16.905	15.087	50.644	1.00	14.49
ATOM	2070	O	LEU	B	71	16.270	15.031	51.692	1.00	17.54
ATOM	2071	N	ALA	B	72	18.205	15.358	50.615	1.00	14.25
ATOM	2072	CA	ALA	B	72	18.983	15.648	51.835	1.00	9.02
ATOM	2073	CB	ALA	B	72	19.533	14.373	52.408	1.00	6.95
ATOM	2074	C	ALA	B	72	20.149	16.582	51.565	1.00	10.37
ATOM	2075	O	ALA	B	72	20.841	16.534	50.559	1.00	14.80
ATOM	2076	N	VAL	B	73	20.378	17.432	52.536	1.00	11.58
ATOM	2077	CA	VAL	B	73	21.486	18.367	52.511	1.00	12.95
ATOM	2078	CB	VAL	B	73	20.988	19.808	52.370	1.00	9.61
ATOM	2079	CG1	VAL	B	73	22.170	20.765	52.334	1.00	4.74

Fig. 400

ATOM	2080	CG2	VAL	B	73	20.124	19.935	51.132	1.00	3.64
ATOM	2081	C	VAL	B	73	22.064	18.169	53.936	1.00	18.32
ATOM	2082	O	VAL	B	73	21.401	18.437	54.937	1.00	22.65
ATOM	2083	N	VAL	B	74	23.262	17.596	54.026	1.00	21.86
ATOM	2084	CA	VAL	B	74	23.948	17.375	55.341	1.00	18.90
ATOM	2085	CB	VAL	B	74	24.442	15.935	55.497	1.00	21.15
ATOM	2086	CG1	VAL	B	74	25.246	15.811	56.788	1.00	25.84
ATOM	2087	CG2	VAL	B	74	23.267	14.934	55.462	1.00	22.63
ATOM	2088	C	VAL	B	74	25.200	18.281	55.418	1.00	21.01
ATOM	2089	O	VAL	B	74	25.985	18.410	54.486	1.00	26.38
ATOM	2090	N	ASN	B	75	25.384	18.926	56.550	1.00	21.49
ATOM	2091	CA	ASN	B	75	26.554	19.791	56.728	1.00	21.46
ATOM	2092	CB	ASN	B	75	26.263	20.794	57.835	1.00	22.08
ATOM	2093	CG	ASN	B	75	27.355	21.817	58.007	1.00	24.47
ATOM	2094	OD1	ASN	B	75	27.152	22.825	58.682	1.00	27.48
ATOM	2095	ND2	ASN	B	75	28.520	21.580	57.409	1.00	24.10
ATOM	2096	C	ASN	B	75	27.779	18.909	57.060	1.00	26.34
ATOM	2097	O	ASN	B	75	27.976	18.461	58.193	1.00	34.33
ATOM	2098	N	ASP	B	76	28.569	18.613	56.030	1.00	25.27
ATOM	2099	CA	ASP	B	76	29.809	17.800	56.175	1.00	18.30
ATOM	2100	CB	ASP	B	76	30.186	17.176	54.815	1.00	19.72
ATOM	2101	CG	ASP	B	76	31.430	16.260	54.879	1.00	18.03
ATOM	2102	OD1	ASP	B	76	32.568	16.762	54.802	1.00	20.83
ATOM	2103	OD2	ASP	B	76	31.283	15.027	54.978	1.00	21.41
ATOM	2104	C	ASP	B	76	30.898	18.777	56.644	1.00	19.11
ATOM	2105	O	ASP	B	76	30.821	19.998	56.435	1.00	20.23
ATOM	2106	N	PRO	B	77	31.931	18.245	57.313	1.00	17.61
ATOM	2107	CD	PRO	B	77	32.017	16.869	57.841	1.00	15.76
ATOM	2108	CA	PRO	B	77	33.041	19.054	57.804	1.00	12.96
ATOM	2109	CB	PRO	B	77	34.045	18.003	58.217	1.00	14.74
ATOM	2110	CG	PRO	B	77	33.182	16.959	58.802	1.00	19.87
ATOM	2111	C	PRO	B	77	33.639	19.917	56.697	1.00	15.83
ATOM	2112	O	PRO	B	77	34.258	20.955	56.959	1.00	16.48
ATOM	2113	N	ARG	B	78	33.461	19.451	55.453	1.00	16.28
ATOM	2114	CA	ARG	B	78	34.011	20.129	54.221	1.00	15.16
ATOM	2115	CB	ARG	B	78	34.440	19.081	53.176	1.00	19.75
ATOM	2116	CG	ARG	B	78	35.498	18.054	53.674	1.00	27.41
ATOM	2117	CD	ARG	B	78	35.938	17.071	52.590	1.00	27.76
ATOM	2118	NE	ARG	B	78	36.547	17.759	51.445	1.00	34.10
ATOM	2119	CZ	ARG	B	78	36.347	17.430	50.169	1.00	35.08
ATOM	2120	NH1	ARG	B	78	36.948	18.120	49.211	1.00	33.35
ATOM	2121	NH2	ARG	B	78	35.557	16.410	49.844	1.00	35.93
ATOM	2122	C	ARG	B	78	33.101	21.161	53.565	1.00	12.35
ATOM	2123	O	ARG	B	78	33.578	22.095	52.943	1.00	15.66
ATOM	2124	N	GLY	B	79	31.789	20.964	53.677	1.00	10.86
ATOM	2125	CA	GLY	B	79	30.831	21.881	53.088	1.00	11.07
ATOM	2126	C	GLY	B	79	29.470	21.225	53.031	1.00	13.88
ATOM	2127	O	GLY	B	79	29.358	20.025	53.310	1.00	16.49
ATOM	2128	N	PRO	B	80	28.405	21.973	52.700	1.00	12.83
ATOM	2129	CD	PRO	B	80	28.428	23.394	52.305	1.00	11.83
ATOM	2130	CA	PRO	B	80	27.045	21.419	52.616	1.00	7.71
ATOM	2131	CB	PRO	B	80	26.201	22.639	52.336	1.00	8.81

Fig. 4PP

ATOM	2132	CG	PRO	B	80	27.125	23.512	51.531	1.00	10.78
ATOM	2133	C	PRO	B	80	26.940	20.470	51.444	1.00	12.29
ATOM	2134	O	PRO	B	80	26.977	20.874	50.290	1.00	14.42
ATOM	2135	N	PHE	B	81	26.742	19.196	51.757	1.00	13.09
ATOM	2136	CA	PHE	B	81	26.626	18.109	50.747	1.00	13.43
ATOM	2137	CB	PHE	B	81	27.368	16.892	51.304	1.00	10.32
ATOM	2138	CG	PHE	B	81	27.441	15.719	50.368	1.00	10.20
ATOM	2139	CD1	PHE	B	81	28.426	15.654	49.388	1.00	11.18
ATOM	2140	CD2	PHE	B	81	26.573	14.636	50.518	1.00	9.80
ATOM	2141	CE1	PHE	B	81	28.550	14.519	48.571	1.00	12.48
ATOM	2142	CE2	PHE	B	81	26.688	13.500	49.708	1.00	6.35
ATOM	2143	CZ	PHE	B	81	27.677	13.439	48.737	1.00	8.16
ATOM	2144	C	PHE	B	81	25.128	17.814	50.489	1.00	15.88
ATOM	2145	O	PHE	B	81	24.280	17.997	51.361	1.00	21.18
ATOM	2146	N	PHE	B	82	24.788	17.370	49.282	1.00	14.59
ATOM	2147	CA	PHE	B	82	23.370	17.067	48.999	1.00	10.94
ATOM	2148	CB	PHE	B	82	22.674	18.267	48.369	1.00	12.56
ATOM	2149	CG	PHE	B	82	22.612	18.215	46.873	1.00	14.05
ATOM	2150	CD1	PHE	B	82	23.734	18.531	46.101	1.00	12.10
ATOM	2151	CD2	PHE	B	82	21.434	17.844	46.226	1.00	11.75
ATOM	2152	CE1	PHE	B	82	23.682	18.476	44.698	1.00	8.37
ATOM	2153	CE2	PHE	B	82	21.377	17.787	44.818	1.00	13.13
ATOM	2154	CZ	PHE	B	82	22.499	18.101	44.061	1.00	5.89
ATOM	2155	C	PHE	B	82	23.183	15.838	48.137	1.00	10.61
ATOM	2156	O	PHE	B	82	24.093	15.286	47.534	1.00	12.70
ATOM	2157	N	VAL	B	83	21.964	15.358	48.152	1.00	10.54
ATOM	2158	CA	VAL	B	83	21.608	14.212	47.342	1.00	14.69
ATOM	2159	CB	VAL	B	83	21.587	12.936	48.162	1.00	13.77
ATOM	2160	CG1	VAL	B	83	20.946	11.822	47.388	1.00	11.74
ATOM	2161	CG2	VAL	B	83	22.991	12.530	48.454	1.00	17.05
ATOM	2162	C	VAL	B	83	20.217	14.581	46.831	1.00	17.90
ATOM	2163	O	VAL	B	83	19.359	15.033	47.600	1.00	23.98
ATOM	2164	N	GLY	B	84	20.038	14.491	45.514	1.00	14.79
ATOM	2165	CA	GLY	B	84	18.769	14.825	44.901	1.00	11.59
ATOM	2166	C	GLY	B	84	18.288	13.725	43.991	1.00	11.44
ATOM	2167	O	GLY	B	84	19.056	12.814	43.659	1.00	17.85
ATOM	2168	N	LEU	B	85	17.038	13.839	43.549	1.00	10.95
ATOM	2169	CA	LEU	B	85	16.394	12.847	42.665	1.00	6.95
ATOM	2170	CB	LEU	B	85	15.241	12.189	43.400	1.00	11.44
ATOM	2171	CG	LEU	B	85	14.380	11.197	42.628	1.00	11.93
ATOM	2172	CD1	LEU	B	85	15.159	9.934	42.493	1.00	14.60
ATOM	2173	CD2	LEU	B	85	13.109	10.900	43.383	1.00	13.51
ATOM	2174	C	LEU	B	85	15.861	13.575	41.473	1.00	7.78
ATOM	2175	O	LEU	B	85	15.188	14.581	41.597	1.00	8.59
ATOM	2176	N	ILE	B	86	16.111	13.008	40.304	1.00	10.44
ATOM	2177	CA	ILE	B	86	15.648	13.557	39.027	1.00	6.43
ATOM	2178	CB	ILE	B	86	16.846	13.856	38.127	1.00	6.56
ATOM	2179	CG2	ILE	B	86	16.395	14.379	36.777	1.00	5.68
ATOM	2180	CG1	ILE	B	86	17.739	14.879	38.794	1.00	5.33
ATOM	2181	CD1	ILE	B	86	18.995	15.090	38.022	1.00	2.81
ATOM	2182	C	ILE	B	86	14.787	12.461	38.361	1.00	10.78
ATOM	2183	O	ILE	B	86	15.263	11.361	38.032	1.00	13.27

Fig. 4QQ

ATOM	2184	N	ALA	B	87	13.502	12.760	38.194	1.00	9.91
ATOM	2185	CA	ALA	B	87	12.536	11.812	37.567	1.00	10.38
ATOM	2186	CB	ALA	B	87	11.536	11.331	38.600	1.00	14.06
ATOM	2187	C	ALA	B	87	11.820	12.610	36.484	1.00	13.06
ATOM	2188	O	ALA	B	87	10.779	13.224	36.703	1.00	15.63
ATOM	2189	N	CYS	B	88	12.402	12.607	35.293	1.00	13.93
ATOM	2190	CA	CYS	B	88	11.852	13.389	34.180	1.00	8.89
ATOM	2191	CB	CYS	B	88	12.505	14.754	34.209	1.00	2.00
ATOM	2192	SG	CYS	B	88	11.912	15.969	33.027	1.00	9.78
ATOM	2193	C	CYS	B	88	12.186	12.638	32.916	1.00	11.99
ATOM	2194	O	CYS	B	88	13.331	12.437	32.575	1.00	19.71
ATOM	2195	N	VAL	B	89	11.153	12.177	32.230	1.00	14.28
ATOM	2196	CA	VAL	B	89	11.328	11.417	30.995	1.00	10.90
ATOM	2197	CB	VAL	B	89	10.095	10.542	30.723	1.00	13.28
ATOM	2198	CG1	VAL	B	89	8.908	11.408	30.329	1.00	16.79
ATOM	2199	CG2	VAL	B	89	10.399	9.509	29.649	1.00	12.90
ATOM	2200	C	VAL	B	89	11.573	12.342	29.798	1.00	10.81
ATOM	2201	O	VAL	B	89	12.216	11.988	28.814	1.00	13.96
ATOM	2202	N	GLN	B	90	11.066	13.558	29.882	1.00	9.74
ATOM	2203	CA	GLN	B	90	11.258	14.514	28.762	1.00	12.71
ATOM	2204	CB	GLN	B	90	10.403	15.756	29.001	1.00	9.68
ATOM	2205	CG	GLN	B	90	8.934	15.394	29.138	1.00	16.94
ATOM	2206	CD	GLN	B	90	8.003	16.576	29.272	1.00	14.86
ATOM	2207	OE1	GLN	B	90	8.310	17.554	29.950	1.00	18.44
ATOM	2208	NE2	GLN	B	90	6.851	16.486	28.631	1.00	16.05
ATOM	2209	C	GLN	B	90	12.761	14.852	28.634	1.00	16.58
ATOM	2210	O	GLN	B	90	13.355	14.838	27.558	1.00	22.11
ATOM	2211	N	LEU	B	91	13.373	15.142	29.777	1.00	17.96
ATOM	2212	CA	LEU	B	91	14.820	15.468	29.847	1.00	16.95
ATOM	2213	CB	LEU	B	91	15.232	15.623	31.305	1.00	14.75
ATOM	2214	CG	LEU	B	91	16.687	15.866	31.647	1.00	9.95
ATOM	2215	CD1	LEU	B	91	17.189	17.038	30.863	1.00	6.41
ATOM	2216	CD2	LEU	B	91	16.768	16.137	33.124	1.00	9.30
ATOM	2217	C	LEU	B	91	15.585	14.330	29.167	1.00	16.51
ATOM	2218	O	LEU	B	91	16.450	14.552	28.320	1.00	22.78
ATOM	2219	N	GLU	B	92	15.206	13.101	29.512	1.00	14.86
ATOM	2220	CA	GLU	B	92	15.820	11.896	28.922	1.00	14.75
ATOM	2221	CB	GLU	B	92	15.166	10.624	29.432	1.00	15.36
ATOM	2222	CG	GLU	B	92	15.345	10.351	30.904	1.00	18.69
ATOM	2223	CD	GLU	B	92	14.586	9.114	31.342	1.00	23.90
ATOM	2224	OE1	GLU	B	92	14.000	9.179	32.437	1.00	24.57
ATOM	2225	OE2	GLU	B	92	14.557	8.098	30.592	1.00	25.95
ATOM	2226	C	GLU	B	92	15.714	11.914	27.400	1.00	18.59
ATOM	2227	O	GLU	B	92	16.712	11.826	26.703	1.00	24.00
ATOM	2228	N	ARG	B	93	14.490	12.027	26.885	1.00	18.28
ATOM	2229	CA	ARG	B	93	14.262	12.030	25.410	1.00	18.13
ATOM	2230	CB	ARG	B	93	12.767	12.036	25.076	1.00	24.10
ATOM	2231	CG	ARG	B	93	11.937	10.990	25.808	1.00	33.78
ATOM	2232	CD	ARG	B	93	12.345	9.557	25.486	1.00	43.31
ATOM	2233	NE	ARG	B	93	11.589	8.611	26.318	1.00	53.94
ATOM	2234	CZ	ARG	B	93	11.570	7.285	26.158	1.00	57.23
ATOM	2235	NH1	ARG	B	93	10.848	6.530	26.986	1.00	53.37

Fig. 4RR

ATOM	2236	NH2	ARG	B	93	12.253	6.714	25.165	1.00	60.34
ATOM	2237	C	ARG	B	93	14.955	13.193	24.695	1.00	15.47
ATOM	2238	O	ARG	B	93	15.576	13.022	23.644	1.00	14.08
ATOM	2239	N	VAL	B	94	14.837	14.383	25.281	1.00	12.48
ATOM	2240	CA	VAL	B	94	15.451	15.600	24.715	1.00	13.20
ATOM	2241	CB	VAL	B	94	15.119	16.836	25.579	1.00	14.89
ATOM	2242	CG1	VAL	B	94	16.033	18.001	25.219	1.00	11.53
ATOM	2243	CG2	VAL	B	94	13.676	17.262	25.323	1.00	10.23
ATOM	2244	C	VAL	B	94	16.986	15.417	24.542	1.00	15.57
ATOM	2245	O	VAL	B	94	17.595	15.752	23.508	1.00	18.39
ATOM	2246	N	LEU	B	95	17.591	14.841	25.575	1.00	12.07
ATOM	2247	CA	LEU	B	95	19.037	14.542	25.593	1.00	10.59
ATOM	2248	CB	LEU	B	95	19.416	14.207	27.031	1.00	9.22
ATOM	2249	CG	LEU	B	95	20.509	14.994	27.749	1.00	13.75
ATOM	2250	CD1	LEU	B	95	20.535	16.434	27.319	1.00	7.90
ATOM	2251	CD2	LEU	B	95	20.291	14.877	29.247	1.00	9.99
ATOM	2252	C	LEU	B	95	19.388	13.354	24.613	1.00	13.40
ATOM	2253	O	LEU	B	95	20.270	13.430	23.755	1.00	10.88
ATOM	2254	N	GLU	B	96	18.661	12.252	24.768	1.00	13.38
ATOM	2255	CA	GLU	B	96	18.857	11.034	23.955	1.00	15.22
ATOM	2256	CB	GLU	B	96	17.811	9.973	24.312	1.00	24.43
ATOM	2257	CG	GLU	B	96	18.132	9.005	25.442	1.00	32.00
ATOM	2258	CD	GLU	B	96	16.951	8.078	25.783	1.00	38.78
ATOM	2259	OE1	GLU	B	96	16.967	7.484	26.887	1.00	50.86
ATOM	2260	OE2	GLU	B	96	16.005	7.935	24.969	1.00	38.36
ATOM	2261	C	GLU	B	96	18.750	11.326	22.470	1.00	15.80
ATOM	2262	O	GLU	B	96	19.446	10.735	21.638	1.00	19.07
ATOM	2263	N	THR	B	97	17.806	12.197	22.128	1.00	13.25
ATOM	2264	CA	THR	B	97	17.586	12.513	20.713	1.00	10.33
ATOM	2265	CB	THR	B	97	16.135	12.953	20.403	1.00	9.54
ATOM	2266	OG1	THR	B	97	15.856	14.186	21.055	1.00	13.77
ATOM	2267	CG2	THR	B	97	15.137	11.901	20.886	1.00	12.86
ATOM	2268	C	THR	B	97	18.553	13.531	20.196	1.00	10.29
ATOM	2269	O	THR	B	97	18.862	13.541	19.021	1.00	15.13
ATOM	2270	N	ALA	B	98	19.028	14.423	21.062	1.00	10.23
ATOM	2271	CA	ALA	B	98	20.006	15.437	20.591	1.00	9.69
ATOM	2272	CB	ALA	B	98	20.293	16.497	21.664	1.00	6.19
ATOM	2273	C	ALA	B	98	21.287	14.691	20.225	1.00	10.63
ATOM	2274	O	ALA	B	98	21.950	14.975	19.242	1.00	11.46
ATOM	2275	N	ALA	B	99	21.629	13.709	21.041	1.00	13.55
ATOM	2276	CA	ALA	B	99	22.837	12.940	20.802	1.00	17.54
ATOM	2277	CB	ALA	B	99	23.216	12.100	22.008	1.00	17.11
ATOM	2278	C	ALA	B	99	22.697	12.049	19.585	1.00	24.87
ATOM	2279	O	ALA	B	99	22.138	10.955	19.603	1.00	23.85
ATOM	2280	N	SER	B	100	23.271	12.550	18.502	1.00	35.12
ATOM	2281	CA	SER	B	100	23.369	11.828	17.208	1.00	41.56
ATOM	2282	CB	SER	B	100	23.480	12.835	16.055	1.00	44.46
ATOM	2283	OG	SER	B	100	22.410	13.783	16.065	1.00	48.22
ATOM	2284	C	SER	B	100	24.730	11.150	17.494	1.00	44.46
ATOM	2285	O	SER	B	100	25.722	11.263	16.767	1.00	42.45
ATOM	2286	N	ALA	B	101	24.733	10.497	18.655	1.00	50.25
ATOM	2287	CA	ALA	B	101	25.895	9.829	19.237	1.00	54.69

Fig. 4SS

ATOM	2288	CB	ALA B 101	25.552	9.300	20.649	1.00	53.60
ATOM	2289	C	ALA B 101	26.542	8.731	18.407	1.00	58.50
ATOM	2290	O	ALA B 101	25.905	7.853	17.793	1.00	57.09
ATOM	2291	N	ALA B 102	27.864	8.865	18.376	1.00	62.77
ATOM	2292	CA	ALA B 102	28.768	7.919	17.722	1.00	66.11
ATOM	2293	CB	ALA B 102	30.030	8.650	17.241	1.00	63.86
ATOM	2294	C	ALA B 102	29.088	7.024	18.943	1.00	69.14
ATOM	2295	O	ALA B 102	28.790	5.825	19.011	1.00	73.52
ATOM	2296	N	ALA B 103	29.629	7.680	19.960	1.00	68.90
ATOM	2297	CA	ALA B 103	29.976	7.015	21.222	1.00	69.10
ATOM	2298	CB	ALA B 103	31.329	6.264	21.096	1.00	68.74
ATOM	2299	C	ALA B 103	30.049	8.142	22.273	1.00	69.15
ATOM	2300	O	ALA B 103	30.027	7.796	23.477	1.00	72.07
ATOM	2301	OT	ALA B 103	30.051	9.341	21.870	1.00	63.18
ATOM	2302	CB	ALA B 111	28.451	2.056	27.380	1.00	59.43
ATOM	2303	C	ALA B 111	26.410	1.110	26.192	1.00	55.79
ATOM	2304	O	ALA B 111	26.484	0.178	25.387	1.00	54.99
ATOM	2305	N	ALA B 111	26.884	3.629	26.299	1.00	58.71
ATOM	2306	CA	ALA B 111	27.463	2.259	26.220	1.00	57.49
ATOM	2307	N	SER B 112	25.409	1.222	27.063	1.00	54.21
ATOM	2308	CA	SER B 112	24.357	0.190	27.187	1.00	53.07
ATOM	2309	CB	SER B 112	24.571	-0.601	28.475	1.00	58.33
ATOM	2310	OG	SER B 112	25.759	-1.384	28.425	1.00	65.13
ATOM	2311	C	SER B 112	22.910	0.636	27.121	1.00	49.91
ATOM	2312	O	SER B 112	22.121	0.098	26.358	1.00	54.68
ATOM	2313	N	ARG B 113	22.544	1.613	27.944	1.00	44.84
ATOM	2314	CA	ARG B 113	21.124	2.055	27.986	1.00	43.03
ATOM	2315	CB	ARG B 113	20.332	0.903	28.581	1.00	52.72
ATOM	2316	CG	ARG B 113	21.173	0.043	29.575	1.00	63.19
ATOM	2317	CD	ARG B 113	20.340	-0.560	30.717	1.00	73.93
ATOM	2318	NE	ARG B 113	19.096	-1.183	30.253	1.00	79.97
ATOM	2319	CZ	ARG B 113	17.913	-0.573	30.244	1.00	81.34
ATOM	2320	NH1	ARG B 113	16.838	-1.216	29.802	1.00	83.78
ATOM	2321	NH2	ARG B 113	17.807	0.682	30.670	1.00	82.16
ATOM	2322	C	ARG B 113	20.944	3.340	28.799	1.00	39.66
ATOM	2323	O	ARG B 113	21.194	4.445	28.347	1.00	39.63
ATOM	2324	N	GLU B 114	20.497	3.182	30.037	1.00	38.77
ATOM	2325	CA	GLU B 114	20.349	4.340	30.942	1.00	38.18
ATOM	2326	CB	GLU B 114	19.572	3.946	32.198	1.00	40.24
ATOM	2327	CG	GLU B 114	20.183	2.798	32.978	1.00	46.21
ATOM	2328	CD	GLU B 114	19.173	1.710	33.339	1.00	53.55
ATOM	2329	OE1	GLU B 114	17.950	1.886	33.105	1.00	58.82
ATOM	2330	OE2	GLU B 114	19.610	0.663	33.863	1.00	57.09
ATOM	2331	C	GLU B 114	21.784	4.824	31.269	1.00	34.03
ATOM	2332	O	GLU B 114	22.022	5.888	31.825	1.00	34.98
ATOM	2333	N	GLU B 115	22.754	3.994	30.921	1.00	26.68
ATOM	2334	CA	GLU B 115	24.151	4.377	31.108	1.00	26.38
ATOM	2335	CB	GLU B 115	25.049	3.167	30.961	1.00	29.70
ATOM	2336	CG	GLU B 115	25.107	2.344	32.240	1.00	39.85
ATOM	2337	CD	GLU B 115	25.270	0.851	31.992	1.00	47.81
ATOM	2338	OE1	GLU B 115	26.235	0.479	31.278	1.00	44.94
ATOM	2339	OE2	GLU B 115	24.436	0.055	32.520	1.00	50.33

Fig. 4TT

ATOM	2340	C	GLU B 115	24.452	5.441	30.060	1.00	23.31
ATOM	2341	O	GLU B 115	25.182	6.393	30.281	1.00	23.55
ATOM	2342	N	ARG B 116	23.849	5.281	28.892	1.00	21.14
ATOM	2343	CA	ARG B 116	24.038	6.287	27.839	1.00	20.64
ATOM	2344	CB	ARG B 116	23.265	5.943	26.563	1.00	22.82
ATOM	2345	CG	ARG B 116	24.133	5.471	25.379	1.00	36.84
ATOM	2346	CD	ARG B 116	24.145	6.427	24.114	1.00	48.10
ATOM	2347	NE	ARG B 116	25.173	7.478	24.130	1.00	46.21
ATOM	2348	CZ	ARG B 116	26.394	7.402	23.600	1.00	47.41
ATOM	2349	NH1	ARG B 116	27.194	8.432	23.736	1.00	51.35
ATOM	2350	NH2	ARG B 116	26.824	6.347	22.921	1.00	49.43
ATOM	2351	C	ARG B 116	23.478	7.560	28.468	1.00	19.84
ATOM	2352	O	ARG B 116	24.095	8.618	28.473	1.00	22.78
ATOM	2353	N	LEU B 117	22.297	7.430	29.057	1.00	17.65
ATOM	2354	CA	LEU B 117	21.652	8.589	29.686	1.00	14.89
ATOM	2355	CB	LEU B 117	20.301	8.154	30.269	1.00	16.14
ATOM	2356	CG	LEU B 117	19.548	9.053	31.252	1.00	13.05
ATOM	2357	CD1	LEU B 117	19.351	10.447	30.699	1.00	9.32
ATOM	2358	CD2	LEU B 117	18.222	8.408	31.528	1.00	14.86
ATOM	2359	C	LEU B 117	22.598	9.209	30.747	1.00	15.06
ATOM	2360	O	LEU B 117	22.827	10.420	30.797	1.00	16.67
ATOM	2361	N	LEU B 118	23.199	8.348	31.559	1.00	14.24
ATOM	2362	CA	LEU B 118	24.101	8.819	32.618	1.00	10.27
ATOM	2363	CB	LEU B 118	24.618	7.629	33.413	1.00	8.73
ATOM	2364	CG	LEU B 118	23.938	7.334	34.757	1.00	8.30
ATOM	2365	CD1	LEU B 118	22.884	8.393	35.069	1.00	9.57
ATOM	2366	CD2	LEU B 118	23.336	5.948	34.739	1.00	7.43
ATOM	2367	C	LEU B 118	25.242	9.592	31.980	1.00	11.84
ATOM	2368	O	LEU B 118	25.566	10.738	32.309	1.00	11.94
ATOM	2369	N	TYR B 119	25.809	8.954	30.978	1.00	11.03
ATOM	2370	CA	TYR B 119	26.925	9.533	30.237	1.00	14.62
ATOM	2371	CB	TYR B 119	27.317	8.573	29.134	1.00	17.95
ATOM	2372	CG	TYR B 119	28.343	9.171	28.232	1.00	29.23
ATOM	2373	CD1	TYR B 119	27.960	9.966	27.142	1.00	32.82
ATOM	2374	CE1	TYR B 119	28.905	10.542	26.298	1.00	39.16
ATOM	2375	CD2	TYR B 119	29.698	8.965	28.463	1.00	30.58
ATOM	2376	CE2	TYR B 119	30.656	9.534	27.626	1.00	39.63
ATOM	2377	CZ	TYR B 119	30.255	10.321	26.544	1.00	41.40
ATOM	2378	OH	TYR B 119	31.205	10.886	25.715	1.00	48.04
ATOM	2379	C	TYR B 119	26.625	10.941	29.667	1.00	12.82
ATOM	2380	O	TYR B 119	27.423	11.875	29.713	1.00	15.87
ATOM	2381	N	LEU B 120	25.453	11.062	29.083	1.00	10.54
ATOM	2382	CA	LEU B 120	25.010	12.329	28.499	1.00	9.76
ATOM	2383	CB	LEU B 120	23.736	12.067	27.685	1.00	9.66
ATOM	2384	CG	LEU B 120	23.730	12.114	26.155	1.00	7.96
ATOM	2385	CD1	LEU B 120	25.119	11.872	25.618	1.00	9.33
ATOM	2386	CD2	LEU B 120	22.727	11.087	25.603	1.00	5.94
ATOM	2387	C	LEU B 120	24.790	13.471	29.535	1.00	9.78
ATOM	2388	O	LEU B 120	25.348	14.561	29.453	1.00	12.23
ATOM	2389	N	ILE B 121	23.986	13.206	30.551	1.00	8.55
ATOM	2390	CA	ILE B 121	23.699	14.267	31.512	1.00	2.58
ATOM	2391	CB	ILE B 121	22.502	13.921	32.427	1.00	5.92

Fig. 40U

ATOM	2392	CG2	ILE B 121	22.923	12.978	33.566	1.00	4.29
ATOM	2393	CG1	ILE B 121	21.897	15.213	32.968	1.00	5.94
ATOM	2394	CD1	ILE B 121	20.636	15.010	33.721	1.00	7.70
ATOM	2395	C	ILE B 121	24.927	14.641	32.294	1.00	2.01
ATOM	2396	O	ILE B 121	25.235	15.816	32.489	1.00	3.56
ATOM	2397	N	THR B 122	25.699	13.633	32.677	1.00	7.14
ATOM	2398	CA	THR B 122	26.937	13.890	33.461	1.00	6.03
ATOM	2399	CB	THR B 122	27.757	12.625	33.724	1.00	2.00
ATOM	2400	OG1	THR B 122	26.933	11.632	34.307	1.00	2.00
ATOM	2401	CG2	THR B 122	28.846	12.928	34.723	1.00	2.65
ATOM	2402	C	THR B 122	27.861	14.904	32.760	1.00	6.41
ATOM	2403	O	THR B 122	28.281	15.908	33.327	1.00	9.16
ATOM	2404	N	ASN B 123	28.133	14.663	31.485	1.00	9.14
ATOM	2405	CA	ASN B 123	29.047	15.568	30.734	1.00	8.97
ATOM	2406	CB	ASN B 123	29.724	14.817	29.596	1.00	11.34
ATOM	2407	CG	ASN B 123	30.535	13.668	30.094	1.00	12.46
ATOM	2408	OD1	ASN B 123	30.200	12.504	29.858	1.00	14.50
ATOM	2409	ND2	ASN B 123	31.562	13.975	30.864	1.00	9.02
ATOM	2410	C	ASN B 123	28.420	16.846	30.235	1.00	8.15
ATOM	2411	O	ASN B 123	29.119	17.806	29.923	1.00	9.35
ATOM	2412	N	TYR B 124	27.091	16.849	30.113	1.00	10.17
ATOM	2413	CA	TYR B 124	26.386	18.070	29.652	1.00	5.76
ATOM	2414	CB	TYR B 124	25.099	17.742	28.912	1.00	2.67
ATOM	2415	CG	TYR B 124	24.617	18.911	28.060	1.00	5.33
ATOM	2416	CD1	TYR B 124	25.295	19.281	26.893	1.00	7.28
ATOM	2417	CE1	TYR B 124	24.905	20.398	26.147	1.00	8.26
ATOM	2418	CD2	TYR B 124	23.527	19.690	28.451	1.00	6.81
ATOM	2419	CE2	TYR B 124	23.130	20.823	27.711	1.00	8.31
ATOM	2420	CZ	TYR B 124	23.821	21.165	26.566	1.00	7.58
ATOM	2421	OH	TYR B 124	23.438	22.266	25.855	1.00	5.26
ATOM	2422	C	TYR B 124	26.125	19.036	30.813	1.00	8.01
ATOM	2423	O	TYR B 124	26.336	20.238	30.688	1.00	13.58
ATOM	2424	N	LEU B 125	25.669	18.507	31.946	1.00	4.43
ATOM	2425	CA	LEU B 125	25.399	19.345	33.142	1.00	7.35
ATOM	2426	CB	LEU B 125	23.909	19.294	33.471	1.00	4.74
ATOM	2427	CG	LEU B 125	22.920	19.822	32.432	1.00	4.85
ATOM	2428	CD1	LEU B 125	21.551	19.196	32.631	1.00	2.00
ATOM	2429	CD2	LEU B 125	22.863	21.326	32.472	1.00	2.81
ATOM	2430	C	LEU B 125	26.250	18.775	34.306	1.00	8.86
ATOM	2431	O	LEU B 125	25.761	18.107	35.203	1.00	16.80
ATOM	2432	N	PRO B 126	27.549	19.045	34.298	1.00	8.94
ATOM	2433	CD	PRO B 126	28.339	19.724	33.259	1.00	11.24
ATOM	2434	CA	PRO B 126	28.414	18.529	35.353	1.00	7.93
ATOM	2435	CB	PRO B 126	29.776	18.529	34.676	1.00	9.38
ATOM	2436	CG	PRO B 126	29.723	19.774	33.872	1.00	8.61
ATOM	2437	C	PRO B 126	28.444	19.283	36.684	1.00	8.73
ATOM	2438	O	PRO B 126	28.940	18.765	37.672	1.00	15.99
ATOM	2439	N	SER B 127	27.874	20.478	36.742	1.00	7.51
ATOM	2440	CA	SER B 127	27.882	21.253	38.015	1.00	9.27
ATOM	2441	CB	SER B 127	28.693	22.527	37.796	1.00	12.59
ATOM	2442	OG	SER B 127	29.906	22.231	37.129	1.00	17.76
ATOM	2443	C	SER B 127	26.520	21.609	38.660	1.00	11.04
ATOM	2444	O	SER B 127	25.460	21.548	38.028	1.00	9.89

Fig. 4VV

ATOM	2445	N	VAL B 128	26.578	21.971	39.949	1.00	9.43
ATOM	2446	CA	VAL B 128	25.371	22.410	40.724	1.00	7.72
ATOM	2447	CB	VAL B 128	25.120	21.722	42.112	1.00	7.63
ATOM	2448	CG1	VAL B 128	24.281	20.498	41.949	1.00	15.58
ATOM	2449	CG2	VAL B 128	26.391	21.435	42.850	1.00	2.00
ATOM	2450	C	VAL B 128	25.607	23.849	41.052	1.00	5.88
ATOM	2451	O	VAL B 128	26.729	24.334	41.076	1.00	6.74
ATOM	2452	P1	SEI B 129	25.519	29.079	40.400	1.00	14.99
ATOM	2453	O3	SEI B 129	25.766	29.247	38.832	1.00	11.58
ATOM	2454	O4	SEI B 129	25.075	30.510	40.988	1.00	14.48
ATOM	2455	O5	SEI B 129	24.304	28.037	40.705	1.00	8.14
ATOM	2456	C5	SEI B 129	24.906	29.836	37.866	1.00	20.86
ATOM	2457	C6	SEI B 129	25.585	31.039	37.220	1.00	19.82
ATOM	2458	C7	SEI B 129	24.473	28.793	36.826	1.00	23.22
ATOM	2459	C8	SEI B 129	24.682	30.827	42.313	1.00	9.79
ATOM	2460	C9	SEI B 129	23.385	31.636	42.292	1.00	12.60
ATOM	2461	C10	SEI B 129	25.813	31.584	42.978	1.00	13.43
ATOM	2462	N	SEI B 129	24.523	24.505	41.414	1.00	3.64
ATOM	2463	CA	SEI B 129	24.573	25.896	41.749	1.00	5.61
ATOM	2464	C	SEI B 129	23.438	26.120	42.741	1.00	7.34
ATOM	2465	O	SEI B 129	22.271	25.854	42.468	1.00	12.17
ATOM	2466	CB	SEI B 129	24.351	26.648	40.458	1.00	2.00
ATOM	2467	O2	SEI B 129	26.762	28.599	41.046	1.00	14.25
ATOM	2468	N	LEU B 130	23.807	26.510	43.952	1.00	4.55
ATOM	2469	CA	LEU B 130	22.814	26.749	45.005	1.00	6.57
ATOM	2470	CB	LEU B 130	23.325	26.339	46.377	1.00	10.22
ATOM	2471	CG	LEU B 130	22.435	26.812	47.537	1.00	10.59
ATOM	2472	CD1	LEU B 130	21.219	25.911	47.708	1.00	6.47
ATOM	2473	CD2	LEU B 130	23.245	26.840	48.811	1.00	17.62
ATOM	2474	C	LEU B 130	22.467	28.178	45.059	1.00	6.26
ATOM	2475	O	LEU B 130	23.325	29.026	45.206	1.00	6.59
ATOM	2476	N	SER B 131	21.183	28.465	44.924	1.00	11.26
ATOM	2477	CA	SER B 131	20.728	29.862	45.027	1.00	13.28
ATOM	2478	CB	SER B 131	19.569	30.160	44.082	1.00	13.17
ATOM	2479	OG	SER B 131	20.000	30.148	42.743	1.00	17.83
ATOM	2480	C	SER B 131	20.285	30.029	46.470	1.00	13.30
ATOM	2481	O	SER B 131	19.729	29.103	47.082	1.00	14.83
ATOM	2482	N	THR B 132	20.617	31.190	47.026	1.00	14.68
ATOM	2483	CA	THR B 132	20.238	31.558	48.411	1.00	23.27
ATOM	2484	CB	THR B 132	21.453	31.820	49.285	1.00	18.86
ATOM	2485	OG1	THR B 132	22.336	32.710	48.602	1.00	22.21
ATOM	2486	CG2	THR B 132	22.163	30.536	49.584	1.00	18.49
ATOM	2487	C	THR B 132	19.441	32.871	48.316	1.00	30.52
ATOM	2488	O	THR B 132	19.774	33.755	47.511	1.00	34.88
ATOM	2489	N	ALA B 133	18.374	32.965	49.114	1.00	34.31
ATOM	2490	CA	ALA B 133	17.491	34.164	49.141	1.00	37.83
ATOM	2491	CB	ALA B 133	16.179	33.825	49.850	1.00	37.10
ATOM	2492	C	ALA B 133	18.196	35.371	49.833	1.00	43.25
ATOM	2493	O	ALA B 133	18.153	36.511	49.285	1.00	46.91
ATOM	2494	OT	ALA B 133	18.801	35.145	50.910	1.00	47.08
ATOM	2495	CB	ALA B 141	21.810	32.816	58.328	1.00	39.82
ATOM	2496	C	ALA B 141	19.477	32.765	59.227	1.00	37.50

Fig. 4WW

ATOM	2497	O	ALA B 141	19.419	32.695	60.452	1.00	39.73
ATOM	2498	N	ALA B 141	20.876	34.800	59.432	1.00	40.30
ATOM	2499	CA	ALA B 141	20.552	33.638	58.556	1.00	39.18
ATOM	2500	N	ASP B 142	18.619	32.131	58.418	1.00	35.54
ATOM	2501	CA	ASP B 142	17.542	31.222	58.939	1.00	34.78
ATOM	2502	CB	ASP B 142	16.287	32.015	59.305	1.00	40.40
ATOM	2503	CG	ASP B 142	15.499	32.467	58.100	1.00	44.17
ATOM	2504	OD1	ASP B 142	14.584	31.714	57.722	1.00	48.60
ATOM	2505	OD2	ASP B 142	15.768	33.568	57.550	1.00	44.92
ATOM	2506	C	ASP B 142	17.222	30.077	57.948	1.00	33.91
ATOM	2507	O	ASP B 142	17.741	30.025	56.843	1.00	35.30
ATOM	2508	N	ARG B 143	16.322	29.181	58.342	1.00	35.00
ATOM	2509	CA	ARG B 143	15.948	27.979	57.500	1.00	35.88
ATOM	2510	CB	ARG B 143	14.943	27.076	58.251	1.00	40.75
ATOM	2511	CG	ARG B 143	15.146	26.968	59.772	1.00	45.82
ATOM	2512	CD	ARG B 143	15.334	25.538	60.280	1.00	48.09
ATOM	2513	NE	ARG B 143	15.437	25.548	61.745	1.00	60.16
ATOM	2514	CZ	ARG B 143	16.474	25.095	62.465	1.00	63.46
ATOM	2515	NH1	ARG B 143	16.436	25.168	63.795	1.00	63.68
ATOM	2516	NH2	ARG B 143	17.546	24.571	61.878	1.00	63.18
ATOM	2517	C	ARG B 143	15.434	28.240	56.053	1.00	33.76
ATOM	2518	O	ARG B 143	15.241	27.323	55.253	1.00	32.56
ATOM	2519	N	THR B 144	15.214	29.503	55.720	1.00	30.77
ATOM	2520	CA	THR B 144	14.737	29.842	54.366	1.00	28.86
ATOM	2521	CB	THR B 144	13.628	30.887	54.437	1.00	29.22
ATOM	2522	OG1	THR B 144	14.175	32.132	54.893	1.00	27.77
ATOM	2523	CG2	THR B 144	12.556	30.427	55.417	1.00	30.05
ATOM	2524	C	THR B 144	15.866	30.389	53.475	1.00	26.69
ATOM	2525	O	THR B 144	15.629	30.999	52.438	1.00	32.36
ATOM	2526	N	LEU B 145	17.108	30.192	53.896	1.00	22.02
ATOM	2527	CA	LEU B 145	18.258	30.708	53.109	1.00	20.99
ATOM	2528	CB	LEU B 145	19.537	30.629	53.951	1.00	19.79
ATOM	2529	CG	LEU B 145	20.848	31.126	53.345	1.00	15.95
ATOM	2530	CD1	LEU B 145	20.842	32.616	53.136	1.00	14.52
ATOM	2531	CD2	LEU B 145	21.947	30.753	54.277	1.00	18.00
ATOM	2532	C	LEU B 145	18.430	29.993	51.739	1.00	19.73
ATOM	2533	O	LEU B 145	18.560	30.611	50.701	1.00	22.38
ATOM	2534	N	PHE B 146	18.431	28.670	51.758	1.00	17.81
ATOM	2535	CA	PHE B 146	18.589	27.868	50.536	1.00	15.34
ATOM	2536	CB	PHE B 146	18.991	26.436	50.905	1.00	13.39
ATOM	2537	CG	PHE B 146	20.370	26.315	51.488	1.00	13.44
ATOM	2538	CD1	PHE B 146	20.870	25.072	51.871	1.00	14.63
ATOM	2539	CD2	PHE B 146	21.165	27.439	51.681	1.00	16.84
ATOM	2540	CE1	PHE B 146	22.135	24.953	52.447	1.00	10.15
ATOM	2541	CE2	PHE B 146	22.438	27.329	52.260	1.00	14.58
ATOM	2542	CZ	PHE B 146	22.917	26.082	52.643	1.00	11.68
ATOM	2543	C	PHE B 146	17.280	27.881	49.749	1.00	15.13
ATOM	2544	O	PHE B 146	16.255	27.384	50.182	1.00	18.59
ATOM	2545	N	ALA B 147	17.341	28.453	48.558	1.00	17.08
ATOM	2546	CA	ALA B 147	16.154	28.562	47.642	1.00	18.51
ATOM	2547	CB	ALA B 147	16.265	29.844	46.815	1.00	20.19
ATOM	2548	C	ALA B 147	15.965	27.334	46.682	1.00	19.37

Fig. 4XX

ATOM	2549	O	ALA	B	147	14.880	26.755	46.536	1.00	23.52
ATOM	2550	N	HIS	B	148	17.026	26.999	45.958	1.00	13.42
ATOM	2551	CA	HIS	B	148	16.974	25.862	45.037	1.00	10.50
ATOM	2552	CB	HIS	B	148	15.975	26.133	43.917	1.00	9.04
ATOM	2553	CG	HIS	B	148	16.284	27.361	43.115	1.00	13.85
ATOM	2554	CD2	HIS	B	148	15.926	28.653	43.289	1.00	16.64
ATOM	2555	ND1	HIS	B	148	17.061	27.329	41.973	1.00	22.27
ATOM	2556	CE1	HIS	B	148	17.169	28.549	41.479	1.00	16.08
ATOM	2557	NE2	HIS	B	148	16.488	29.371	42.257	1.00	20.15
ATOM	2558	C	HIS	B	148	18.364	25.626	44.474	1.00	11.93
ATOM	2559	O	HIS	B	148	19.283	26.423	44.672	1.00	12.97
ATOM	2560	N	VAL	B	149	18.505	24.497	43.787	1.00	11.22
ATOM	2561	CA	VAL	B	149	19.759	24.115	43.140	1.00	10.27
ATOM	2562	CB	VAL	B	149	20.396	22.811	43.717	1.00	11.51
ATOM	2563	CG1	VAL	B	149	20.208	22.760	45.208	1.00	14.24
ATOM	2564	CG2	VAL	B	149	19.851	21.566	43.072	1.00	11.24
ATOM	2565	C	VAL	B	149	19.460	23.942	41.663	1.00	11.83
ATOM	2566	O	VAL	B	149	18.419	23.426	41.222	1.00	13.37
ATOM	2567	N	ALA	B	150	20.406	24.434	40.885	1.00	12.95
ATOM	2568	CA	ALA	B	150	20.324	24.392	39.438	1.00	9.02
ATOM	2569	CB	ALA	B	150	20.402	25.795	38.904	1.00	11.66
ATOM	2570	C	ALA	B	150	21.482	23.565	38.871	1.00	8.97
ATOM	2571	O	ALA	B	150	22.632	23.709	39.275	1.00	12.77
ATOM	2572	N	LEU	B	151	21.150	22.626	37.995	1.00	7.32
ATOM	2573	CA	LEU	B	151	22.177	21.822	37.314	1.00	3.63
ATOM	2574	CB	LEU	B	151	21.561	20.574	36.701	1.00	8.28
ATOM	2575	CG	LEU	B	151	21.249	19.340	37.586	1.00	13.08
ATOM	2576	CD1	LEU	B	151	21.148	19.677	39.058	1.00	10.08
ATOM	2577	CD2	LEU	B	151	19.985	18.634	37.094	1.00	12.45
ATOM	2578	C	LEU	B	151	22.671	22.801	36.240	1.00	4.77
ATOM	2579	O	LEU	B	151	21.957	23.681	35.748	1.00	6.86
ATOM	2580	N	CYS	B	152	23.952	22.741	35.964	1.00	6.25
ATOM	2581	CA	CYS	B	152	24.513	23.639	34.967	1.00	6.17
ATOM	2582	CB	CYS	B	152	24.644	25.033	35.551	1.00	2.00
ATOM	2583	SG	CYS	B	152	25.638	25.054	37.012	1.00	17.14
ATOM	2584	C	CYS	B	152	25.855	23.079	34.512	1.00	5.89
ATOM	2585	O	CYS	B	152	26.315	22.044	34.989	1.00	8.57
ATOM	2586	N	ALA	B	153	26.434	23.747	33.522	1.00	5.41
ATOM	2587	CA	ALA	B	153	27.707	23.364	32.928	1.00	4.87
ATOM	2588	CB	ALA	B	153	27.887	24.108	31.626	1.00	2.96
ATOM	2589	C	ALA	B	153	28.880	23.682	33.856	1.00	9.92
ATOM	2590	O	ALA	B	153	29.752	22.864	34.138	1.00	11.99
ATOM	2591	N	ILE	B	154	28.901	24.921	34.312	1.00	8.95
ATOM	2592	CA	ILE	B	154	29.978	25.394	35.164	1.00	13.64
ATOM	2593	CB	ILE	B	154	31.059	26.154	34.275	1.00	20.80
ATOM	2594	CG2	ILE	B	154	32.190	26.719	35.116	1.00	22.34
ATOM	2595	CG1	ILE	B	154	31.695	25.205	33.247	1.00	22.54
ATOM	2596	CD1	ILE	B	154	32.481	24.047	33.853	1.00	28.65
ATOM	2597	C	ILE	B	154	29.319	26.326	36.219	1.00	12.91
ATOM	2598	O	ILE	B	154	28.628	27.298	35.900	1.00	13.79
ATOM	2599	N	GLY	B	155	29.506	25.965	37.490	1.00	16.22
ATOM	2600	CA	GLY	B	155	28.950	26.726	38.611	1.00	14.51

Fig. 4YY

ATOM	2601	C	GLY	B	155	29.881	27.842	39.041	1.00	11.98
ATOM	2602	O	GLY	B	155	30.999	27.908	38.594	1.00	14.71
ATOM	2603	N	ARG	B	156	29.455	28.716	39.926	1.00	13.56
ATOM	2604	CA	ARG	B	156	30.346	29.826	40.309	1.00	14.30
ATOM	2605	CB	ARG	B	156	29.531	31.107	40.414	1.00	14.73
ATOM	2606	CG	ARG	B	156	28.786	31.396	39.149	1.00	22.12
ATOM	2607	CD	ARG	B	156	28.610	32.866	38.948	1.00	35.28
ATOM	2608	NE	ARG	B	156	28.027	33.502	40.121	1.00	48.94
ATOM	2609	CZ	ARG	B	156	28.245	34.769	40.462	1.00	56.23
ATOM	2610	NH1	ARG	B	156	27.668	35.266	41.553	1.00	60.17
ATOM	2611	NH2	ARG	B	156	29.040	35.541	39.722	1.00	59.06
ATOM	2612	C	ARG	B	156	31.168	29.578	41.569	1.00	13.08
ATOM	2613	O	ARG	B	156	32.069	30.330	41.930	1.00	12.46
ATOM	2614	N	ARG	B	157	30.803	28.515	42.265	1.00	13.13
ATOM	2615	CA	ARG	B	157	31.485	28.148	43.496	1.00	11.72
ATOM	2616	CB	ARG	B	157	30.472	27.872	44.624	1.00	12.67
ATOM	2617	CG	ARG	B	157	29.704	29.114	45.117	1.00	9.87
ATOM	2618	CD	ARG	B	157	29.266	28.984	46.588	1.00	13.32
ATOM	2619	NE	ARG	B	157	27.818	28.843	46.786	1.00	20.09
ATOM	2620	CZ	ARG	B	157	26.946	29.855	46.884	1.00	19.55
ATOM	2621	NH1	ARG	B	157	25.678	29.651	47.094	1.00	23.95
ATOM	2622	NH2	ARG	B	157	27.291	31.084	46.652	1.00	23.51
ATOM	2623	C	ARG	B	157	32.337	26.930	43.173	1.00	10.92
ATOM	2624	O	ARG	B	157	32.011	26.103	42.321	1.00	6.72
ATOM	2625	N	LEU	B	158	33.465	26.851	43.865	1.00	10.73
ATOM	2626	CA	LEU	B	158	34.431	25.752	43.668	1.00	8.72
ATOM	2627	CB	LEU	B	158	35.741	26.081	44.379	1.00	10.73
ATOM	2628	CG	LEU	B	158	36.829	26.934	43.726	1.00	10.53
ATOM	2629	CD1	LEU	B	158	36.305	27.648	42.506	1.00	10.03
ATOM	2630	CD2	LEU	B	158	37.385	27.921	44.753	1.00	6.05
ATOM	2631	C	LEU	B	158	33.888	24.425	44.171	1.00	9.08
ATOM	2632	O	LEU	B	158	32.939	24.353	44.936	1.00	11.24
ATOM	2633	N	GLY	B	159	34.526	23.359	43.708	1.00	10.66
ATOM	2634	CA	GLY	B	159	34.160	22.016	44.108	1.00	7.71
ATOM	2635	C	GLY	B	159	32.758	21.581	43.779	1.00	8.04
ATOM	2636	O	GLY	B	159	32.347	20.492	44.164	1.00	10.92
ATOM	2637	N	THR	B	160	32.031	22.393	43.030	1.00	10.18
ATOM	2638	CA	THR	B	160	30.649	22.048	42.678	1.00	11.25
ATOM	2639	CB	THR	B	160	29.810	23.307	42.479	1.00	10.87
ATOM	2640	OG1	THR	B	160	30.463	24.164	41.526	1.00	4.27
ATOM	2641	CG2	THR	B	160	29.639	24.014	43.816	1.00	7.08
ATOM	2642	C	THR	B	160	30.513	21.159	41.436	1.00	11.94
ATOM	2643	O	THR	B	160	29.957	21.517	40.419	1.00	16.34
ATOM	2644	N	ILE	B	161	31.064	19.974	41.519	1.00	11.86
ATOM	2645	CA	ILE	B	161	30.943	19.036	40.424	1.00	11.50
ATOM	2646	CB	ILE	B	161	32.337	18.564	39.970	1.00	8.85
ATOM	2647	CG2	ILE	B	161	32.231	17.379	39.003	1.00	10.76
ATOM	2648	CG1	ILE	B	161	33.044	19.713	39.269	1.00	5.36
ATOM	2649	CD1	ILE	B	161	32.336	20.177	38.021	1.00	6.51
ATOM	2650	C	ILE	B	161	30.100	17.911	41.069	1.00	16.51
ATOM	2651	O	ILE	B	161	30.333	17.461	42.202	1.00	18.10
ATOM	2652	N	VAL	B	162	29.055	17.506	40.369	1.00	16.97

Fig. 4ZZ

ATOM	2653	CA	VAL B 162	28.172	16.468	40.905	1.00	14.97
ATOM	2654	CB	VAL B 162	26.688	16.890	40.825	1.00	15.28
ATOM	2655	CG1	VAL B 162	26.508	18.215	41.512	1.00	12.92
ATOM	2656	CG2	VAL B 162	26.213	16.941	39.380	1.00	8.32
ATOM	2657	C	VAL B 162	28.341	15.123	40.207	1.00	17.23
ATOM	2658	O	VAL B 162	28.947	14.994	39.151	1.00	20.63
ATOM	2659	N	THR B 163	27.742	14.112	40.822	1.00	18.18
ATOM	2660	CA	THR B 163	27.756	12.734	40.317	1.00	15.19
ATOM	2661	CB	THR B 163	28.394	11.777	41.385	1.00	15.60
ATOM	2662	OG1	THR B 163	29.773	12.123	41.592	1.00	12.70
ATOM	2663	CG2	THR B 163	28.327	10.333	40.952	1.00	16.80
ATOM	2664	C	THR B 163	26.271	12.355	40.080	1.00	14.87
ATOM	2665	O	THR B 163	25.345	12.800	40.770	1.00	19.32
ATOM	2666	N	TYR B 164	26.054	11.557	39.051	1.00	9.64
ATOM	2667	CA	TYR B 164	24.721	11.096	38.715	1.00	5.61
ATOM	2668	CB	TYR B 164	24.367	11.578	37.321	1.00	7.77
ATOM	2669	CG	TYR B 164	24.194	13.065	37.161	1.00	5.11
ATOM	2670	CD1	TYR B 164	25.215	13.849	36.673	1.00	6.64
ATOM	2671	CE1	TYR B 164	25.023	15.208	36.425	1.00	4.55
ATOM	2672	CD2	TYR B 164	22.975	13.669	37.409	1.00	3.93
ATOM	2673	CE2	TYR B 164	22.784	15.008	37.158	1.00	5.02
ATOM	2674	CZ	TYR B 164	23.805	15.766	36.664	1.00	2.00
ATOM	2675	OH	TYR B 164	23.580	17.068	36.352	1.00	2.00
ATOM	2676	C	TYR B 164	24.740	9.561	38.718	1.00	10.82
ATOM	2677	O	TYR B 164	25.729	8.939	38.349	1.00	13.25
ATOM	2678	N	ASP B 165	23.662	8.937	39.173	1.00	12.08
ATOM	2679	CA	ASP B 165	23.587	7.465	39.102	1.00	13.24
ATOM	2680	CB	ASP B 165	24.603	6.802	40.026	1.00	16.40
ATOM	2681	CG	ASP B 165	25.297	5.623	39.352	1.00	20.71
ATOM	2682	OD1	ASP B 165	24.624	4.621	39.032	1.00	22.41
ATOM	2683	OD2	ASP B 165	26.518	5.705	39.113	1.00	26.52
ATOM	2684	C	ASP B 165	22.161	6.990	39.376	1.00	15.45
ATOM	2685	O	ASP B 165	21.294	7.755	39.783	1.00	16.33
ATOM	2686	N	THR B 166	21.898	5.722	39.080	1.00	16.15
ATOM	2687	CA	THR B 166	20.543	5.138	39.293	1.00	18.39
ATOM	2688	CB	THR B 166	20.300	4.018	38.329	1.00	15.26
ATOM	2689	OG1	THR B 166	21.350	3.072	38.496	1.00	16.28
ATOM	2690	CG2	THR B 166	20.330	4.531	36.901	1.00	14.97
ATOM	2691	C	THR B 166	20.334	4.559	40.704	1.00	22.40
ATOM	2692	O	THR B 166	19.372	3.843	40.965	1.00	27.49
ATOM	2693	N	SER B 167	21.278	4.849	41.599	1.00	25.31
ATOM	2694	CA	SER B 167	21.235	4.386	43.007	1.00	21.41
ATOM	2695	CB	SER B 167	21.929	3.012	43.159	1.00	27.45
ATOM	2696	OG	SER B 167	23.065	3.031	44.032	1.00	28.47
ATOM	2697	C	SER B 167	21.944	5.471	43.804	1.00	21.42
ATOM	2698	O	SER B 167	22.947	6.055	43.380	1.00	21.57
ATOM	2699	N	LEU B 168	21.363	5.788	44.949	1.00	23.05
ATOM	2700	CA	LEU B 168	21.920	6.819	45.863	1.00	22.96
ATOM	2701	CB	LEU B 168	21.001	6.980	47.078	1.00	19.41
ATOM	2702	CG	LEU B 168	21.393	7.936	48.192	1.00	14.69
ATOM	2703	CD1	LEU B 168	20.191	8.226	48.975	1.00	12.83
ATOM	2704	CD2	LEU B 168	22.443	7.346	49.093	1.00	23.19

Fig. 4AAA

ATOM	2705	C	LEU B 168	23.324	6.400	46.283	1.00	23.29
ATOM	2706	O	LEU B 168	24.266	7.181	46.247	1.00	26.87
ATOM	2707	N	ASP B 169	23.439	5.131	46.674	1.00	25.84
ATOM	2708	CA	ASP B 169	24.725	4.536	47.112	1.00	25.99
ATOM	2709	CB	ASP B 169	24.505	3.071	47.507	1.00	28.63
ATOM	2710	CG	ASP B 169	24.140	2.916	48.992	1.00	34.54
ATOM	2711	OD1	ASP B 169	24.574	1.919	49.616	1.00	36.98
ATOM	2712	OD2	ASP B 169	23.441	3.801	49.544	1.00	33.74
ATOM	2713	C	ASP B 169	25.807	4.680	46.045	1.00	25.28
ATOM	2714	O	ASP B 169	26.968	4.998	46.322	1.00	27.41
ATOM	2715	N	ALA B 170	25.380	4.513	44.796	1.00	26.04
ATOM	2716	CA	ALA B 170	26.292	4.635	43.607	1.00	24.21
ATOM	2717	CB	ALA B 170	25.596	4.072	42.355	1.00	22.04
ATOM	2718	C	ALA B 170	26.715	6.111	43.353	1.00	20.70
ATOM	2719	O	ALA B 170	27.846	6.435	42.980	1.00	21.57
ATOM	2720	N	ALA B 171	25.754	6.996	43.575	1.00	16.12
ATOM	2721	CA	ALA B 171	25.942	8.412	43.366	1.00	12.56
ATOM	2722	CB	ALA B 171	24.589	9.105	43.365	1.00	11.02
ATOM	2723	C	ALA B 171	26.888	9.045	44.394	1.00	16.48
ATOM	2724	O	ALA B 171	27.554	10.042	44.125	1.00	20.58
ATOM	2725	N	ILE B 172	26.936	8.482	45.598	1.00	19.83
ATOM	2726	CA	ILE B 172	27.846	9.039	46.658	1.00	20.98
ATOM	2727	CB	ILE B 172	27.134	9.158	48.043	1.00	25.13
ATOM	2728	CG2	ILE B 172	25.662	9.517	47.842	1.00	28.72
ATOM	2729	CG1	ILE B 172	27.243	7.856	48.849	1.00	27.28
ATOM	2730	CD1	ILE B 172	26.580	7.931	50.237	1.00	27.33
ATOM	2731	C	ILE B 172	29.235	8.306	46.794	1.00	17.41
ATOM	2732	O	ILE B 172	30.213	8.843	47.328	1.00	15.53
ATOM	2733	N	ALA B 173	29.310	7.093	46.253	1.00	10.44
ATOM	2734	CA	ALA B 173	30.558	6.298	46.295	1.00	12.32
ATOM	2735	CB	ALA B 173	30.375	5.005	45.560	1.00	12.15
ATOM	2736	C	ALA B 173	31.823	7.014	45.765	1.00	12.79
ATOM	2737	O	ALA B 173	32.882	6.896	46.348	1.00	17.71
ATOM	2738	N	PRO B 174	31.728	7.747	44.634	1.00	11.72
ATOM	2739	CD	PRO B 174	30.618	7.960	43.690	1.00	5.96
ATOM	2740	CA	PRO B 174	32.933	8.417	44.144	1.00	7.36
ATOM	2741	CB	PRO B 174	32.442	9.117	42.882	1.00	5.91
ATOM	2742	CG	PRO B 174	31.353	8.224	42.429	1.00	6.53
ATOM	2743	C	PRO B 174	33.459	9.439	45.140	1.00	10.22
ATOM	2744	O	PRO B 174	34.609	9.864	45.094	1.00	14.59
ATOM	2745	N	PHE B 175	32.589	9.892	46.029	1.00	12.76
ATOM	2746	CA	PHE B 175	33.022	10.890	47.035	1.00	18.32
ATOM	2747	CB	PHE B 175	31.809	11.687	47.513	1.00	17.04
ATOM	2748	CG	PHE B 175	31.260	12.618	46.466	1.00	11.91
ATOM	2749	CD1	PHE B 175	31.751	13.913	46.348	1.00	7.73
ATOM	2750	CD2	PHE B 175	30.290	12.182	45.571	1.00	8.77
ATOM	2751	CE1	PHE B 175	31.290	14.755	45.350	1.00	6.39
ATOM	2752	CE2	PHE B 175	29.821	13.011	44.572	1.00	2.00
ATOM	2753	CZ	PHE B 175	30.318	14.298	44.457	1.00	6.14
ATOM	2754	C	PHE B 175	33.822	10.264	48.211	1.00	23.77
ATOM	2755	O	PHE B 175	33.298	9.785	49.216	1.00	24.51
ATOM	2756	N	ARG B 176	35.139	10.307	48.056	1.00	29.90

Fig. 48BB

ATOM	2757	CA	ARG B 176	36.091	9.732	49.053	1.00	31.16
ATOM	2758	CB	ARG B 176	37.381	9.362	48.299	1.00	32.42
ATOM	2759	CG	ARG B 176	37.138	8.411	47.097	1.00	33.93
ATOM	2760	CD	ARG B 176	36.568	7.051	47.572	1.00	36.16
ATOM	2761	NE	ARG B 176	35.781	6.325	46.565	1.00	39.27
ATOM	2762	CZ	ARG B 176	36.288	5.678	45.513	1.00	42.32
ATOM	2763	NH1	ARG B 176	35.475	5.046	44.660	1.00	39.59
ATOM	2764	NH2	ARG B 176	37.605	5.665	45.299	1.00	46.87
ATOM	2765	C	ARG B 176	36.380	10.610	50.316	1.00	34.51
ATOM	2766	O	ARG B 176	36.590	10.134	51.435	1.00	33.36
ATOM	2767	N	HIS B 177	36.416	11.919	50.127	1.00	37.74
ATOM	2768	CA	HIS B 177	36.685	12.816	51.289	1.00	41.97
ATOM	2769	CB	HIS B 177	37.487	14.027	50.811	1.00	49.15
ATOM	2770	CG	HIS B 177	38.742	13.662	50.070	1.00	57.94
ATOM	2771	CD2	HIS B 177	39.484	14.360	49.175	1.00	60.33
ATOM	2772	ND1	HIS B 177	39.362	12.433	50.204	1.00	60.45
ATOM	2773	CE1	HIS B 177	40.428	12.391	49.425	1.00	60.67
ATOM	2774	NE2	HIS B 177	40.525	13.546	48.790	1.00	62.60
ATOM	2775	C	HIS B 177	35.338	13.217	51.928	1.00	41.22
ATOM	2776	O	HIS B 177	34.963	14.399	52.037	1.00	39.27
ATOM	2777	N	LEU B 178	34.608	12.186	52.350	1.00	35.75
ATOM	2778	CA	LEU B 178	33.270	12.393	52.930	1.00	33.62
ATOM	2779	CB	LEU B 178	32.214	11.781	52.009	1.00	25.56
ATOM	2780	CG	LEU B 178	30.966	12.640	51.850	1.00	23.73
ATOM	2781	CD1	LEU B 178	31.352	13.996	51.246	1.00	17.64
ATOM	2782	CD2	LEU B 178	29.940	11.895	50.987	1.00	20.17
ATOM	2783	C	LEU B 178	33.179	11.793	54.328	1.00	35.50
ATOM	2784	O	LEU B 178	33.387	10.586	54.532	1.00	35.12
ATOM	2785	N	ASP B 179	32.857	12.658	55.292	1.00	33.15
ATOM	2786	CA	ASP B 179	32.739	12.228	56.702	1.00	34.50
ATOM	2787	CB	ASP B 179	32.269	13.376	57.595	1.00	34.37
ATOM	2788	CG	ASP B 179	32.556	13.119	59.069	1.00	35.10
ATOM	2789	OD1	ASP B 179	31.979	12.181	59.660	1.00	35.71
ATOM	2790	OD2	ASP B 179	33.383	13.857	59.645	1.00	40.00
ATOM	2791	C	ASP B 179	31.769	11.054	56.789	1.00	34.54
ATOM	2792	O	ASP B 179	30.656	11.083	56.272	1.00	39.56
ATOM	2793	N	PRO B 180	32.197	9.981	57.450	1.00	33.13
ATOM	2794	CD	PRO B 180	33.550	9.735	57.977	1.00	33.10
ATOM	2795	CA	PRO B 180	31.354	8.796	57.597	1.00	32.32
ATOM	2796	CB	PRO B 180	32.124	7.983	58.631	1.00	30.87
ATOM	2797	CG	PRO B 180	33.540	8.234	58.191	1.00	33.69
ATOM	2798	C	PRO B 180	29.913	9.112	58.041	1.00	29.22
ATOM	2799	O	PRO B 180	28.943	8.490	57.611	1.00	30.25
ATOM	2800	N	ALA B 181	29.798	10.116	58.902	1.00	28.96
ATOM	2801	CA	ALA B 181	28.488	10.560	59.444	1.00	28.30
ATOM	2802	CB	ALA B 181	28.708	11.633	60.515	1.00	26.43
ATOM	2803	C	ALA B 181	27.589	11.098	58.310	1.00	27.73
ATOM	2804	O	ALA B 181	26.377	10.834	58.221	1.00	27.98
ATOM	2805	N	THR B 182	28.228	11.853	57.421	1.00	25.91
ATOM	2806	CA	THR B 182	27.537	12.446	56.259	1.00	24.31
ATOM	2807	CB	THR B 182	28.522	13.235	55.418	1.00	20.96
ATOM	2808	OG1	THR B 182	29.211	14.161	56.276	1.00	19.00

Fig. 4CCC

ATOM	2809	CG2	THR	B	182	27.798	13.969	54.301	1.00	23.44
ATOM	2810	C	THR	B	182	26.852	11.363	55.412	1.00	22.69
ATOM	2811	O	THR	B	182	25.696	11.487	55.037	1.00	22.40
ATOM	2812	N	ARG	B	183	27.562	10.262	55.186	1.00	26.27
ATOM	2813	CA	ARG	B	183	27.030	9.119	54.386	1.00	29.52
ATOM	2814	CB	ARG	B	183	28.121	8.077	54.186	1.00	31.20
ATOM	2815	CG	ARG	B	183	29.339	8.625	53.496	1.00	35.42
ATOM	2816	CD	ARG	B	183	30.325	7.532	53.188	1.00	42.02
ATOM	2817	NE	ARG	B	183	31.455	8.110	52.474	1.00	58.05
ATOM	2818	CZ	ARG	B	183	32.732	7.851	52.742	1.00	64.94
ATOM	2819	NH1	ARG	B	183	33.687	8.450	52.030	1.00	66.47
ATOM	2820	NH2	ARG	B	183	33.062	6.988	53.704	1.00	69.62
ATOM	2821	C	ARG	B	183	25.816	8.475	55.042	1.00	30.12
ATOM	2822	O	ARG	B	183	24.761	8.273	54.442	1.00	32.43
ATOM	2823	N	GLU	B	184	25.979	8.161	56.318	1.00	34.51
ATOM	2824	CA	GLU	B	184	24.897	7.522	57.088	1.00	36.84
ATOM	2825	CB	GLU	B	184	25.424	7.018	58.432	1.00	43.30
ATOM	2826	CG	GLU	B	184	24.648	5.819	58.974	1.00	51.76
ATOM	2827	CD	GLU	B	184	24.342	4.792	57.889	1.00	56.21
ATOM	2828	OE1	GLU	B	184	25.268	4.048	57.473	1.00	56.43
ATOM	2829	OE2	GLU	B	184	23.173	4.755	57.435	1.00	56.35
ATOM	2830	C	GLU	B	184	23.708	8.450	57.281	1.00	33.32
ATOM	2831	O	GLU	B	184	22.564	8.022	57.371	1.00	36.41
ATOM	2832	N	GLY	B	185	23.996	9.743	57.321	1.00	31.11
ATOM	2833	CA	GLY	B	185	22.950	10.729	57.490	1.00	31.01
ATOM	2834	C	GLY	B	185	22.205	11.002	56.200	1.00	33.72
ATOM	2835	O	GLY	B	185	20.963	11.023	56.177	1.00	36.44
ATOM	2836	N	VAL	B	186	22.957	11.151	55.109	1.00	33.46
ATOM	2837	CA	VAL	B	186	22.371	11.451	53.775	1.00	29.64
ATOM	2838	CB	VAL	B	186	23.440	11.923	52.765	1.00	26.92
ATOM	2839	CG1	VAL	B	186	24.057	10.742	52.022	1.00	27.97
ATOM	2840	CG2	VAL	B	186	22.842	12.923	51.838	1.00	20.39
ATOM	2841	C	VAL	B	186	21.570	10.275	53.216	1.00	29.46
ATOM	2842	O	VAL	B	186	20.660	10.441	52.416	1.00	34.31
ATOM	2843	N	ARG	B	187	21.923	9.070	53.642	1.00	30.13
ATOM	2844	CA	ARG	B	187	21.173	7.861	53.209	1.00	32.23
ATOM	2845	CB	ARG	B	187	21.953	6.591	53.527	1.00	32.62
ATOM	2846	CG	ARG	B	187	23.146	6.326	52.666	1.00	32.11
ATOM	2847	CD	ARG	B	187	23.584	4.890	52.872	1.00	34.27
ATOM	2848	NE	ARG	B	187	24.719	4.562	52.020	1.00	41.30
ATOM	2849	CZ	ARG	B	187	25.989	4.673	52.393	1.00	43.96
ATOM	2850	NH1	ARG	B	187	26.955	4.363	51.531	1.00	48.28
ATOM	2851	NH2	ARG	B	187	26.291	5.066	53.630	1.00	45.23
ATOM	2852	C	ARG	B	187	19.822	7.809	53.946	1.00	33.88
ATOM	2853	O	ARG	B	187	18.748	7.577	53.376	1.00	37.83
ATOM	2854	N	ARG	B	188	19.905	8.032	55.251	1.00	32.30
ATOM	2855	CA	ARG	B	188	18.718	7.988	56.126	1.00	35.39
ATOM	2856	CB	ARG	B	188	19.171	8.199	57.568	1.00	40.56
ATOM	2857	CG	ARG	B	188	18.186	7.720	58.609	1.00	48.63
ATOM	2858	CD	ARG	B	188	17.974	8.792	59.679	1.00	56.09
ATOM	2859	NE	ARG	B	188	19.232	9.377	60.152	1.00	59.40
ATOM	2860	CZ	ARG	B	188	19.466	10.687	60.237	1.00	62.01

Fig. 4DDD

ATOM	2861	NH1	ARG	B	188	20.641	11.115	60.677	1.00	62.48
ATOM	2862	NH2	ARG	B	188	18.538	11.572	59.877	1.00	63.45
ATOM	2863	C	ARG	B	188	17.617	8.996	55.720	1.00	33.02
ATOM	2864	O	ARG	B	188	16.448	8.644	55.535	1.00	36.28
ATOM	2865	N	GLU	B	189	17.995	10.265	55.593	1.00	28.51
ATOM	2866	CA	GLU	B	189	17.003	11.300	55.189	1.00	27.26
ATOM	2867	CB	GLU	B	189	17.596	12.699	55.307	1.00	24.81
ATOM	2868	CG	GLU	B	189	18.099	13.014	56.696	1.00	37.35
ATOM	2869	CD	GLU	B	189	18.840	14.337	56.780	1.00	42.32
ATOM	2870	OE1	GLU	B	189	19.800	14.436	57.588	1.00	46.04
ATOM	2871	OE2	GLU	B	189	18.458	15.278	56.044	1.00	48.19
ATOM	2872	C	GLU	B	189	16.480	11.055	53.759	1.00	24.99
ATOM	2873	O	GLU	B	189	15.305	11.192	53.475	1.00	25.77
ATOM	2874	N	ALA	B	190	17.368	10.653	52.861	1.00	26.56
ATOM	2875	CA	ALA	B	190	16.978	10.402	51.457	1.00	26.33
ATOM	2876	CB	ALA	B	190	18.162	9.964	50.668	1.00	24.46
ATOM	2877	C	ALA	B	190	15.845	9.374	51.345	1.00	31.10
ATOM	2878	O	ALA	B	190	14.824	9.611	50.682	1.00	32.33
ATOM	2879	N	ALA	B	191	16.017	8.241	52.031	1.00	31.63
ATOM	2880	CA	ALA	B	191	14.990	7.150	52.034	1.00	32.05
ATOM	2881	CB	ALA	B	191	15.412	6.030	52.979	1.00	31.11
ATOM	2882	C	ALA	B	191	13.607	7.705	52.465	1.00	33.82
ATOM	2883	O	ALA	B	191	12.553	7.457	51.861	1.00	32.73
ATOM	2884	N	GLU	B	192	13.632	8.461	53.555	1.00	35.01
ATOM	2885	CA	GLU	B	192	12.398	9.081	54.086	1.00	36.08
ATOM	2886	CB	GLU	B	192	12.710	9.791	55.413	1.00	38.15
ATOM	2887	CG	GLU	B	192	13.329	8.870	56.477	1.00	46.52
ATOM	2888	CD	GLU	B	192	13.459	9.510	57.862	1.00	53.18
ATOM	2889	OE1	GLU	B	192	13.162	10.726	58.015	1.00	56.34
ATOM	2890	OE2	GLU	B	192	13.870	8.784	58.803	1.00	53.41
ATOM	2891	C	GLU	B	192	11.821	10.056	53.031	1.00	35.97
ATOM	2892	O	GLU	B	192	10.727	9.873	52.493	1.00	36.66
ATOM	2893	N	ALA	B	193	12.626	11.063	52.699	1.00	35.17
ATOM	2894	CA	ALA	B	193	12.263	12.112	51.712	1.00	33.28
ATOM	2895	CB	ALA	B	193	13.493	12.939	51.337	1.00	33.84
ATOM	2896	C	ALA	B	193	11.650	11.497	50.458	1.00	33.19
ATOM	2897	O	ALA	B	193	10.654	11.973	49.919	1.00	32.52
ATOM	2898	N	GLU	B	194	12.250	10.413	49.992	1.00	33.67
ATOM	2899	CA	GLU	B	194	11.716	9.747	48.785	1.00	38.31
ATOM	2900	CB	GLU	B	194	12.557	8.555	48.390	1.00	39.02
ATOM	2901	CG	GLU	B	194	13.656	8.905	47.458	1.00	40.74
ATOM	2902	CD	GLU	B	194	14.380	7.685	47.010	1.00	42.51
ATOM	2903	OE1	GLU	B	194	15.358	7.298	47.698	1.00	49.63
ATOM	2904	OE2	GLU	B	194	13.952	7.102	45.987	1.00	42.55
ATOM	2905	C	GLU	B	194	10.280	9.306	48.966	1.00	40.47
ATOM	2906	O	GLU	B	194	9.454	9.461	48.081	1.00	41.16
ATOM	2907	N	LEU	B	195	9.998	8.732	50.133	1.00	43.06
ATOM	2908	CA	LEU	B	195	8.634	8.257	50.457	1.00	43.16
ATOM	2909	CB	LEU	B	195	8.564	7.832	51.915	1.00	45.19
ATOM	2910	CG	LEU	B	195	9.332	6.543	52.171	1.00	46.09
ATOM	2911	CD1	LEU	B	195	9.084	6.113	53.627	1.00	47.82
ATOM	2912	CD2	LEU	B	195	8.858	5.471	51.175	1.00	45.78

Fig. 4EEE

ATOM	2913	C	LEU B 195	7.547	9.292	50.136	1.00	42.89
ATOM	2914	O	LEU B 195	6.491	8.973	49.597	1.00	43.65
ATOM	2915	N	ALA B 196	7.810	10.545	50.480	1.00	42.64
ATOM	2916	CA	ALA B 196	6.841	11.620	50.178	1.00	45.75
ATOM	2917	CB	ALA B 196	7.308	12.939	50.765	1.00	46.26
ATOM	2918	C	ALA B 196	6.689	11.738	48.639	1.00	47.35
ATOM	2919	O	ALA B 196	5.726	11.266	48.031	1.00	49.97
ATOM	2920	N	LEU B 197	7.694	12.321	47.995	1.00	49.59
ATOM	2921	CA	LEU B 197	7.652	12.488	46.507	1.00	49.86
ATOM	2922	CB	LEU B 197	8.671	13.551	46.049	1.00	41.45
ATOM	2923	CG	LEU B 197	10.184	13.367	46.069	1.00	36.93
ATOM	2924	CD1	LEU B 197	10.576	12.472	47.170	1.00	39.69
ATOM	2925	CD2	LEU B 197	10.671	12.783	44.772	1.00	42.85
ATOM	2926	C	LEU B 197	7.842	11.151	45.762	1.00	51.45
ATOM	2927	O	LEU B 197	8.374	11.073	44.650	1.00	51.60
ATOM	2928	N	ALA B 198	7.380	10.087	46.410	1.00	54.22
ATOM	2929	CA	ALA B 198	7.471	8.730	45.848	1.00	54.54
ATOM	2930	CB	ALA B 198	7.104	7.677	46.896	1.00	59.15
ATOM	2931	C	ALA B 198	6.512	8.652	44.683	1.00	52.43
ATOM	2932	O	ALA B 198	5.288	8.850	44.799	1.00	50.03
ATOM	2933	N	GLY B 199	7.115	8.387	43.530	1.00	48.06
ATOM	2934	CA	GLY B 199	6.353	8.274	42.316	1.00	41.89
ATOM	2935	C	GLY B 199	6.316	9.580	41.562	1.00	37.38
ATOM	2936	O	GLY B 199	6.005	9.562	40.377	1.00	45.85
ATOM	2937	N	ARG B 200	6.642	10.704	42.193	1.00	29.22
ATOM	2938	CA	ARG B 200	6.570	11.970	41.450	1.00	21.98
ATOM	2939	CB	ARG B 200	6.799	13.184	42.337	1.00	20.19
ATOM	2940	CG	ARG B 200	5.767	14.246	42.102	1.00	15.60
ATOM	2941	CD	ARG B 200	6.333	15.483	41.458	1.00	11.83
ATOM	2942	NE	ARG B 200	6.486	16.523	42.466	1.00	12.71
ATOM	2943	CZ	ARG B 200	6.444	17.824	42.217	1.00	10.13
ATOM	2944	NH1	ARG B 200	6.597	18.693	43.204	1.00	14.91
ATOM	2945	NH2	ARG B 200	6.250	18.261	40.991	1.00	7.08
ATOM	2946	C	ARG B 200	7.535	11.962	40.296	1.00	21.16
ATOM	2947	O	ARG B 200	8.650	11.439	40.371	1.00	22.67
ATOM	2948	N	THR B 201	7.029	12.503	39.192	1.00	19.44
ATOM	2949	CA	THR B 201	7.747	12.626	37.911	1.00	13.79
ATOM	2950	CB	THR B 201	7.166	11.682	36.859	1.00	12.91
ATOM	2951	OG1	THR B 201	7.496	10.345	37.219	1.00	17.68
ATOM	2952	CG2	THR B 201	7.746	11.940	35.492	1.00	15.91
ATOM	2953	C	THR B 201	7.457	14.034	37.492	1.00	13.45
ATOM	2954	O	THR B 201	6.321	14.505	37.561	1.00	20.19
ATOM	2955	N	TRP B 202	8.516	14.747	37.137	1.00	11.08
ATOM	2956	CA	TRP B 202	8.389	16.136	36.713	1.00	8.56
ATOM	2957	CB	TRP B 202	9.642	16.890	37.118	1.00	3.97
ATOM	2958	CG	TRP B 202	9.663	17.164	38.589	1.00	2.00
ATOM	2959	CD2	TRP B 202	9.944	16.230	39.636	1.00	2.00
ATOM	2960	CE2	TRP B 202	9.879	16.933	40.849	1.00	2.00
ATOM	2961	CE3	TRP B 202	10.259	14.863	39.667	1.00	3.43
ATOM	2962	CD1	TRP B 202	9.439	18.365	39.194	1.00	2.00
ATOM	2963	NE1	TRP B 202	9.569	18.235	40.549	1.00	2.46
ATOM	2964	CZ2	TRP B 202	10.122	16.325	42.084	1.00	4.01

Fig. 4FFF

ATOM	2965	CZ3	TRP	B	202	10.507	14.249	40.902	1.00	2.00
ATOM	2966	CH2	TRP	B	202	10.435	14.985	42.090	1.00	4.43
ATOM	2967	C	TRP	B	202	8.157	16.158	35.231	1.00	10.04
ATOM	2968	O	TRP	B	202	8.578	15.259	34.514	1.00	17.59
ATOM	2969	N	ALA	B	203	7.442	17.166	34.751	1.00	9.79
ATOM	2970	CA	ALA	B	203	7.180	17.259	33.291	1.00	10.58
ATOM	2971	CB	ALA	B	203	5.858	16.608	32.949	1.00	4.38
ATOM	2972	C	ALA	B	203	7.152	18.723	32.897	1.00	12.21
ATOM	2973	O	ALA	B	203	6.088	19.287	32.658	1.00	11.26
ATOM	2974	N	PRO	B	204	8.342	19.367	32.826	1.00	14.59
ATOM	2975	CD	PRO	B	204	9.688	18.823	33.120	1.00	13.48
ATOM	2976	CA	PRO	B	204	8.420	20.786	32.461	1.00	12.52
ATOM	2977	CB	PRO	B	204	9.909	21.109	32.631	1.00	9.22
ATOM	2978	CG	PRO	B	204	10.600	19.790	32.411	1.00	8.43
ATOM	2979	C	PRO	B	204	7.912	21.127	31.059	1.00	12.04
ATOM	2980	O	PRO	B	204	7.394	22.208	30.816	1.00	14.10
ATOM	2981	N	GLY	B	205	8.021	20.162	30.148	1.00	13.67
ATOM	2982	CA	GLY	B	205	7.615	20.364	28.759	1.00	12.39
ATOM	2983	C	GLY	B	205	8.844	20.287	27.861	1.00	13.93
ATOM	2984	O	GLY	B	205	9.758	21.118	27.946	1.00	16.91
ATOM	2985	N	VAL	B	206	8.857	19.329	26.951	1.00	14.06
ATOM	2986	CA	VAL	B	206	10.023	19.142	26.085	1.00	16.16
ATOM	2987	CB	VAL	B	206	9.819	17.974	25.082	1.00	18.67
ATOM	2988	CG1	VAL	B	206	9.438	16.690	25.810	1.00	16.49
ATOM	2989	CG2	VAL	B	206	8.776	18.327	24.083	1.00	25.86
ATOM	2990	C	VAL	B	206	10.553	20.408	25.373	1.00	17.11
ATOM	2991	O	VAL	B	206	11.756	20.577	25.185	1.00	21.06
ATOM	2992	N	GLU	B	207	9.672	21.320	24.987	1.00	16.09
ATOM	2993	CA	GLU	B	207	10.183	22.530	24.309	1.00	15.16
ATOM	2994	CB	GLU	B	207	9.098	23.249	23.522	1.00	19.15
ATOM	2995	CG	GLU	B	207	8.664	22.478	22.248	1.00	33.99
ATOM	2996	CD	GLU	B	207	9.827	21.763	21.456	1.00	39.72
ATOM	2997	OE1	GLU	B	207	11.010	22.219	21.462	1.00	38.31
ATOM	2998	OE2	GLU	B	207	9.532	20.719	20.815	1.00	39.55
ATOM	2999	C	GLU	B	207	10.874	23.446	25.282	1.00	15.92
ATOM	3000	O	GLU	B	207	11.901	24.041	24.979	1.00	20.22
ATOM	3001	N	ALA	B	208	10.328	23.520	26.493	1.00	12.61
ATOM	3002	CA	ALA	B	208	10.930	24.347	27.559	1.00	10.29
ATOM	3003	CB	ALA	B	208	10.117	24.238	28.796	1.00	6.64
ATOM	3004	C	ALA	B	208	12.345	23.787	27.819	1.00	10.41
ATOM	3005	O	ALA	B	208	13.343	24.498	27.911	1.00	11.42
ATOM	3006	N	LEU	B	209	12.399	22.465	27.893	1.00	7.66
ATOM	3007	CA	LEU	B	209	13.646	21.737	28.107	1.00	7.68
ATOM	3008	CB	LEU	B	209	13.346	20.245	28.262	1.00	6.10
ATOM	3009	CG	LEU	B	209	13.021	19.886	29.711	1.00	4.44
ATOM	3010	CD1	LEU	B	209	12.557	18.493	29.829	1.00	8.65
ATOM	3011	CD2	LEU	B	209	14.260	20.097	30.553	1.00	7.74
ATOM	3012	C	LEU	B	209	14.591	21.990	26.947	1.00	6.98
ATOM	3013	O	LEU	B	209	15.722	22.405	27.094	1.00	13.90
ATOM	3014	N	THR	B	210	14.072	21.812	25.754	1.00	8.48
ATOM	3015	CA	THR	B	210	14.864	22.006	24.572	1.00	6.92
ATOM	3016	CB	THR	B	210	14.061	21.619	23.373	1.00	7.75

Fig. 4GGG

ATOM	3017	OG1	THR	B	210	13.822	20.205	23.429	1.00	12.79
ATOM	3018	CG2	THR	B	210	14.816	21.909	22.119	1.00	12.68
ATOM	3019	C	THR	B	210	15.420	23.432	24.473	1.00	10.25
ATOM	3020	O	THR	B	210	16.585	23.651	24.189	1.00	11.37
ATOM	3021	N	HIS	B	211	14.602	24.415	24.805	1.00	14.19
ATOM	3022	CA	HIS	B	211	15.066	25.811	24.738	1.00	15.90
ATOM	3023	CB	HIS	B	211	13.892	26.778	24.729	1.00	25.74
ATOM	3024	CG	HIS	B	211	13.138	26.799	23.433	1.00	29.51
ATOM	3025	CD2	HIS	B	211	12.182	25.975	22.943	1.00	30.79
ATOM	3026	ND1	HIS	B	211	13.356	27.751	22.461	1.00	36.28
ATOM	3027	CE1	HIS	B	211	12.569	27.515	21.425	1.00	35.36
ATOM	3028	NE2	HIS	B	211	11.846	26.438	21.696	1.00	32.16
ATOM	3029	C	HIS	B	211	16.024	26.155	25.861	1.00	17.72
ATOM	3030	O	HIS	B	211	16.936	26.961	25.710	1.00	23.58
ATOM	3031	N	THR	B	212	15.809	25.551	27.017	1.00	14.16
ATOM	3032	CA	THR	B	212	16.695	25.813	28.151	1.00	9.70
ATOM	3033	CB	THR	B	212	16.078	25.261	29.446	1.00	6.36
ATOM	3034	OG1	THR	B	212	14.850	25.950	29.685	1.00	14.95
ATOM	3035	CG2	THR	B	212	16.966	25.492	30.620	1.00	2.59
ATOM	3036	C	THR	B	212	18.109	25.229	27.881	1.00	8.25
ATOM	3037	O	THR	B	212	19.124	25.903	27.990	1.00	11.25
ATOM	3038	N	LEU	B	213	18.160	23.996	27.424	1.00	2.00
ATOM	3039	CA	LEU	B	213	19.444	23.380	27.182	1.00	5.12
ATOM	3040	CB	LEU	B	213	19.208	21.886	26.953	1.00	7.48
ATOM	3041	CG	LEU	B	213	18.641	21.101	28.146	1.00	3.50
ATOM	3042	CD1	LEU	B	213	18.444	19.656	27.796	1.00	2.00
ATOM	3043	CD2	LEU	B	213	19.588	21.196	29.320	1.00	7.80
ATOM	3044	C	LEU	B	213	20.295	24.071	26.050	1.00	9.49
ATOM	3045	O	LEU	B	213	21.523	24.207	26.135	1.00	15.34
ATOM	3046	N	LEU	B	214	19.625	24.549	25.011	1.00	7.61
ATOM	3047	CA	LEU	B	214	20.329	25.240	23.919	1.00	6.52
ATOM	3048	CB	LEU	B	214	19.356	25.710	22.843	1.00	6.24
ATOM	3049	CG	LEU	B	214	19.844	26.048	21.408	1.00	14.41
ATOM	3050	CD1	LEU	B	214	19.042	27.217	20.841	1.00	2.19
ATOM	3051	CD2	LEU	B	214	21.324	26.373	21.311	1.00	6.72
ATOM	3052	C	LEU	B	214	20.969	26.460	24.572	1.00	6.49
ATOM	3053	O	LEU	B	214	22.113	26.807	24.343	1.00	9.44
ATOM	3054	N	SER	B	215	20.183	27.103	25.417	1.00	4.46
ATOM	3055	CA	SER	B	215	20.607	28.300	26.133	1.00	4.60
ATOM	3056	CB	SER	B	215	19.435	28.754	26.988	1.00	8.67
ATOM	3057	OG	SER	B	215	19.576	30.090	27.411	1.00	21.29
ATOM	3058	C	SER	B	215	21.873	28.006	26.971	1.00	5.38
ATOM	3059	O	SER	B	215	22.814	28.796	27.042	1.00	5.45
ATOM	3060	N	THR	B	216	21.886	26.841	27.599	1.00	5.40
ATOM	3061	CA	THR	B	216	23.004	26.425	28.419	1.00	3.99
ATOM	3062	CB	THR	B	216	22.749	25.037	28.987	1.00	3.17
ATOM	3063	OG1	THR	B	216	21.762	25.144	30.010	1.00	9.54
ATOM	3064	CG2	THR	B	216	24.041	24.422	29.551	1.00	8.72
ATOM	3065	C	THR	B	216	24.216	26.351	27.508	1.00	11.59
ATOM	3066	O	THR	B	216	25.346	26.678	27.876	1.00	16.65
ATOM	3067	N	ALA	B	217	23.959	25.926	26.285	1.00	5.14
ATOM	3068	CA	ALA	B	217	25.026	25.769	25.338	1.00	5.04

Fig. 4HHH

ATOM	3069	CB	ALA	B	217	24.606	24.829	24.241	1.00	6.37
ATOM	3070	C	ALA	B	217	25.493	27.087	24.767	1.00	7.04
ATOM	3071	O	ALA	B	217	26.696	27.355	24.692	1.00	16.59
ATOM	3072	N	VAL	B	218	24.546	27.944	24.401	1.00	3.51
ATOM	3073	CA	VAL	B	218	24.890	29.243	23.804	1.00	4.65
ATOM	3074	CB	VAL	B	218	23.670	29.923	23.183	1.00	2.00
ATOM	3075	CG1	VAL	B	218	24.002	31.334	22.747	1.00	2.00
ATOM	3076	CG2	VAL	B	218	23.229	29.145	21.992	1.00	2.00
ATOM	3077	C	VAL	B	218	25.594	30.198	24.763	1.00	12.31
ATOM	3078	O	VAL	B	218	26.563	30.877	24.412	1.00	20.14
ATOM	3079	N	ASN	B	219	25.131	30.231	26.004	1.00	15.35
ATOM	3080	CA	ASN	B	219	25.741	31.138	27.000	1.00	16.47
ATOM	3081	CB	ASN	B	219	24.752	31.342	28.135	1.00	19.66
ATOM	3082	CG	ASN	B	219	23.492	32.104	27.674	1.00	20.27
ATOM	3083	OD1	ASN	B	219	23.576	33.243	27.216	1.00	25.47
ATOM	3084	ND2	ASN	B	219	22.337	31.462	27.762	1.00	17.30
ATOM	3085	C	ASN	B	219	27.147	30.738	27.493	1.00	16.69
ATOM	3086	O	ASN	B	219	27.916	31.555	27.986	1.00	17.63
ATOM	3087	N	ASN	B	220	27.512	29.482	27.250	1.00	18.59
ATOM	3088	CA	ASN	B	220	28.830	28.977	27.657	1.00	14.92
ATOM	3089	CB	ASN	B	220	28.690	27.694	28.484	1.00	15.29
ATOM	3090	CG	ASN	B	220	28.099	27.947	29.866	1.00	22.86
ATOM	3091	OD1	ASN	B	220	28.824	28.198	30.835	1.00	26.87
ATOM	3092	ND2	ASN	B	220	26.771	27.881	29.964	1.00	24.43
ATOM	3093	C	ASN	B	220	29.739	28.722	26.452	1.00	18.94
ATOM	3094	O	ASN	B	220	30.792	28.088	26.572	1.00	22.85
ATOM	3095	N	MET	B	221	29.355	29.227	25.279	1.00	14.50
ATOM	3096	CA	MET	B	221	30.193	28.982	24.087	1.00	13.78
ATOM	3097	CB	MET	B	221	29.427	29.313	22.810	1.00	11.99
ATOM	3098	CG	MET	B	221	29.037	30.731	22.674	1.00	9.03
ATOM	3099	SD	MET	B	221	28.366	31.026	21.060	1.00	10.14
ATOM	3100	CE	MET	B	221	27.662	32.561	21.311	1.00	2.09
ATOM	3101	C	MET	B	221	31.576	29.678	24.118	1.00	17.08
ATOM	3102	O	MET	B	221	32.580	29.139	23.655	1.00	18.42
ATOM	3103	N	MET	B	222	31.628	30.840	24.765	1.00	20.70
ATOM	3104	CA	MET	B	222	32.886	31.624	24.876	1.00	22.27
ATOM	3105	CB	MET	B	222	32.527	33.097	25.032	1.00	19.96
ATOM	3106	CG	MET	B	222	31.477	33.582	24.027	1.00	24.93
ATOM	3107	SD	MET	B	222	32.024	34.076	22.357	1.00	29.51
ATOM	3108	CE	MET	B	222	32.973	32.716	21.853	1.00	25.54
ATOM	3109	C	MET	B	222	33.842	31.137	26.007	1.00	27.44
ATOM	3110	O	MET	B	222	34.908	31.704	26.280	1.00	31.13
ATOM	3111	N	LEU	B	223	33.456	30.038	26.641	1.00	27.43
ATOM	3112	CA	LEU	B	223	34.257	29.487	27.720	1.00	24.97
ATOM	3113	CB	LEU	B	223	33.440	28.513	28.566	1.00	26.13
ATOM	3114	CG	LEU	B	223	33.811	28.346	30.042	1.00	23.51
ATOM	3115	CD1	LEU	B	223	33.609	29.678	30.724	1.00	28.75
ATOM	3116	CD2	LEU	B	223	32.955	27.280	30.715	1.00	22.72
ATOM	3117	C	LEU	B	223	35.448	28.788	27.121	1.00	27.33
ATOM	3118	O	LEU	B	223	35.341	27.827	26.357	1.00	23.84
ATOM	3119	N	ARG	B	224	36.609	29.344	27.425	1.00	34.22
ATOM	3120	CA	ARG	B	224	37.845	28.738	26.976	1.00	40.95

Fig. 4III

ATOM	3121	CB	ARG	B	224	38.983	29.746	27.045	1.00	46.49
ATOM	3122	CG	ARG	B	224	39.074	30.637	25.822	1.00	53.01
ATOM	3123	CD	ARG	B	224	39.176	29.810	24.544	1.00	58.82
ATOM	3124	NE	ARG	B	224	40.036	30.419	23.526	1.00	69.78
ATOM	3125	CZ	ARG	B	224	39.894	31.654	23.033	1.00	76.79
ATOM	3126	NH1	ARG	B	224	40.746	32.091	22.104	1.00	78.95
ATOM	3127	NH2	ARG	B	224	38.916	32.461	23.461	1.00	79.33
ATOM	3128	C	ARG	B	224	38.118	27.461	27.819	1.00	42.37
ATOM	3129	O	ARG	B	224	38.254	27.433	29.059	1.00	38.17
ATOM	3130	N	ASP	B	225	38.057	26.371	27.073	1.00	47.50
ATOM	3131	CA	ASP	B	225	38.274	25.019	27.567	1.00	51.89
ATOM	3132	CB	ASP	B	225	39.711	24.843	28.082	1.00	62.81
ATOM	3133	CG	ASP	B	225	40.049	23.374	28.411	1.00	69.78
ATOM	3134	OD1	ASP	B	225	40.534	22.610	27.532	1.00	74.02
ATOM	3135	OD2	ASP	B	225	39.833	23.000	29.579	1.00	75.01
ATOM	3136	C	ASP	B	225	37.266	24.412	28.532	1.00	48.26
ATOM	3137	O	ASP	B	225	36.890	23.309	28.312	1.00	53.44
ATOM	3138	N	ARG	B	226	36.844	25.052	29.607	1.00	39.29
ATOM	3139	CA	ARG	B	226	35.833	24.398	30.518	1.00	32.22
ATOM	3140	CB	ARG	B	226	34.452	24.316	29.815	1.00	33.64
ATOM	3141	CG	ARG	B	226	33.913	22.906	29.587	1.00	37.13
ATOM	3142	CD	ARG	B	226	32.493	22.860	29.041	1.00	42.88
ATOM	3143	NE	ARG	B	226	32.013	21.472	29.006	1.00	47.99
ATOM	3144	CZ	ARG	B	226	31.133	20.957	29.862	1.00	47.44
ATOM	3145	NH1	ARG	B	226	30.764	19.687	29.755	1.00	45.94
ATOM	3146	NH2	ARG	B	226	30.608	21.715	30.817	1.00	49.68
ATOM	3147	C	ARG	B	226	36.216	23.024	31.181	1.00	27.95
ATOM	3148	O	ARG	B	226	36.083	22.863	32.390	1.00	30.12
ATOM	3149	N	TRP	B	227	36.677	22.039	30.408	1.00	22.65
ATOM	3150	CA	TRP	B	227	37.075	20.704	30.967	1.00	20.68
ATOM	3151	CB	TRP	B	227	37.407	19.742	29.838	1.00	22.64
ATOM	3152	CG	TRP	B	227	36.172	19.263	29.105	1.00	34.12
ATOM	3153	CD2	TRP	B	227	35.111	18.443	29.636	1.00	37.55
ATOM	3154	CE2	TRP	B	227	34.140	18.299	28.615	1.00	39.86
ATOM	3155	CE3	TRP	B	227	34.888	17.816	30.874	1.00	38.79
ATOM	3156	CD1	TRP	B	227	35.808	19.566	27.813	1.00	33.65
ATOM	3157	NE1	TRP	B	227	34.591	18.992	27.518	1.00	38.20
ATOM	3158	CZ2	TRP	B	227	32.964	17.560	28.796	1.00	37.32
ATOM	3159	CZ3	TRP	B	227	33.716	17.075	31.050	1.00	40.79
ATOM	3160	CH2	TRP	B	227	32.770	16.956	30.011	1.00	40.13
ATOM	3161	C	TRP	B	227	38.211	20.742	31.995	1.00	20.73
ATOM	3162	O	TRP	B	227	38.366	19.853	32.819	1.00	21.16
ATOM	3163	N	SER	B	228	39.025	21.787	31.913	1.00	20.31
ATOM	3164	CA	SER	B	228	40.142	22.013	32.854	1.00	18.99
ATOM	3165	CB	SER	B	228	40.950	23.234	32.453	1.00	22.66
ATOM	3166	OG	SER	B	228	42.107	22.866	31.738	1.00	28.00
ATOM	3167	C	SER	B	228	39.478	22.266	34.184	1.00	18.77
ATOM	3168	O	SER	B	228	39.691	21.548	35.154	1.00	18.92
ATOM	3169	N	LEU	B	229	38.637	23.304	34.198	1.00	16.88
ATOM	3170	CA	LEU	B	229	37.852	23.687	35.400	1.00	13.89
ATOM	3171	CB	LEU	B	229	36.824	24.756	35.072	1.00	14.91
ATOM	3172	CG	LEU	B	229	37.229	25.997	34.302	1.00	21.34

Fig. 4JJJ

ATOM	3173	CD1	LEU	B	229	36.120	27.021	34.437	1.00	25.98
ATOM	3174	CD2	LEU	B	229	38.512	26.562	34.875	1.00	29.24
ATOM	3175	C	LEU	B	229	37.111	22.441	35.927	1.00	14.13
ATOM	3176	O	LEU	B	229	37.150	22.121	37.110	1.00	13.46
ATOM	3177	N	VAL	B	230	36.442	21.718	35.031	1.00	9.92
ATOM	3178	CA	VAL	B	230	35.729	20.525	35.481	1.00	7.86
ATOM	3179	CB	VAL	B	230	34.940	19.839	34.335	1.00	11.57
ATOM	3180	CG1	VAL	B	230	34.352	18.516	34.808	1.00	5.13
ATOM	3181	CG2	VAL	B	230	33.790	20.772	33.848	1.00	6.65
ATOM	3182	C	VAL	B	230	36.728	19.579	36.171	1.00	12.20
ATOM	3183	O	VAL	B	230	36.501	19.140	37.290	1.00	14.24
ATOM	3184	N	ALA	B	231	37.903	19.388	35.569	1.00	15.27
ATOM	3185	CA	ALA	B	231	38.952	18.469	36.156	1.00	13.72
ATOM	3186	CB	ALA	B	231	40.104	18.308	35.205	1.00	9.89
ATOM	3187	C	ALA	B	231	39.470	18.991	37.514	1.00	16.18
ATOM	3188	O	ALA	B	231	39.624	18.273	38.520	1.00	15.14
ATOM	3189	N	GLU	B	232	39.696	20.291	37.553	1.00	13.86
ATOM	3190	CA	GLU	B	232	40.197	20.911	38.784	1.00	15.67
ATOM	3191	CB	GLU	B	232	40.500	22.380	38.549	1.00	19.66
ATOM	3192	CG	GLU	B	232	41.154	22.995	39.754	1.00	25.78
ATOM	3193	CD	GLU	B	232	41.277	24.485	39.680	1.00	28.08
ATOM	3194	OE1	GLU	B	232	41.820	25.041	40.658	1.00	23.63
ATOM	3195	OE2	GLU	B	232	40.831	25.091	38.675	1.00	31.14
ATOM	3196	C	GLU	B	232	39.213	20.779	39.947	1.00	16.23
ATOM	3197	O	GLU	B	232	39.541	20.350	41.062	1.00	16.02
ATOM	3198	N	ARG	B	233	37.969	21.149	39.651	1.00	16.55
ATOM	3199	CA	ARG	B	233	36.896	21.149	40.657	1.00	14.61
ATOM	3200	CB	ARG	B	233	35.764	22.059	40.171	1.00	13.34
ATOM	3201	CG	ARG	B	233	36.345	23.340	39.536	1.00	18.87
ATOM	3202	CD	ARG	B	233	35.810	24.645	40.059	1.00	18.26
ATOM	3203	NE	ARG	B	233	34.477	24.898	39.530	1.00	20.17
ATOM	3204	CZ	ARG	B	233	34.014	26.085	39.147	1.00	17.42
ATOM	3205	NH1	ARG	B	233	32.774	26.170	38.700	1.00	24.17
ATOM	3206	NH2	ARG	B	233	34.771	27.170	39.169	1.00	9.59
ATOM	3207	C	ARG	B	233	36.460	19.738	41.044	1.00	12.43
ATOM	3208	O	ARG	B	233	35.927	19.500	42.114	1.00	14.45
ATOM	3209	N	ARG	B	234	36.781	18.771	40.197	1.00	14.26
ATOM	3210	CA	ARG	B	234	36.459	17.364	40.512	1.00	14.00
ATOM	3211	CB	ARG	B	234	36.632	16.472	39.279	1.00	18.42
ATOM	3212	CG	ARG	B	234	36.450	14.996	39.588	1.00	28.86
ATOM	3213	CD	ARG	B	234	37.005	14.028	38.519	1.00	36.84
ATOM	3214	NE	ARG	B	234	36.946	12.647	39.026	1.00	48.13
ATOM	3215	CZ	ARG	B	234	36.742	11.543	38.297	1.00	50.91
ATOM	3216	NH1	ARG	B	234	36.575	11.591	36.974	1.00	51.01
ATOM	3217	NH2	ARG	B	234	36.639	10.371	38.920	1.00	50.86
ATOM	3218	C	ARG	B	234	37.459	16.962	41.615	1.00	16.26
ATOM	3219	O	ARG	B	234	37.148	16.256	42.579	1.00	16.51
ATOM	3220	N	ARG	B	235	38.688	17.446	41.456	1.00	16.61
ATOM	3221	CA	ARG	B	235	39.767	17.132	42.412	1.00	15.51
ATOM	3222	CB	ARG	B	235	41.110	17.596	41.847	1.00	18.01
ATOM	3223	CG	ARG	B	235	41.476	16.874	40.572	1.00	23.11
ATOM	3224	CD	ARG	B	235	42.908	17.130	40.183	1.00	24.44

Fig. 4KKK

ATOM	3225	NE	ARG	B	235	43.176	18.548	39.996	1.00	27.92
ATOM	3226	C2	ARG	B	235	43.327	19.115	38.806	1.00	30.65
ATOM	3227	NH1	ARG	B	235	43.566	20.426	38.709	1.00	32.71
ATOM	3228	NH2	ARG	B	235	43.237	18.367	37.714	1.00	30.30
ATOM	3229	C	ARG	B	235	39.455	17.766	43.761	1.00	13.89
ATOM	3230	O	ARG	B	235	39.495	17.128	44.818	1.00	12.23
ATOM	3231	N	GLN	B	236	39.108	19.046	43.700	1.00	12.23
ATOM	3232	CA	GLN	B	236	38.729	19.796	44.906	1.00	12.63
ATOM	3233	CB	GLN	B	236	38.224	21.183	44.512	1.00	9.38
ATOM	3234	CG	GLN	B	236	39.239	22.038	43.777	1.00	9.89
ATOM	3235	CD	GLN	B	236	38.610	23.300	43.205	1.00	17.93
ATOM	3236	OE1	GLN	B	236	37.398	23.328	42.933	1.00	22.34
ATOM	3237	NE2	GLN	B	236	39.415	24.355	43.024	1.00	14.90
ATOM	3238	C	GLN	B	236	37.640	19.013	45.706	1.00	15.34
ATOM	3239	O	GLN	B	236	37.746	18.830	46.907	1.00	19.99
ATOM	3240	N	ALA	B	237	36.606	18.529	45.008	1.00	16.40
ATOM	3241	CA	ALA	B	237	35.476	17.777	45.652	1.00	11.75
ATOM	3242	CB	ALA	B	237	34.334	17.576	44.675	1.00	10.37
ATOM	3243	C	ALA	B	237	35.893	16.440	46.200	1.00	14.32
ATOM	3244	O	ALA	B	237	35.192	15.810	46.994	1.00	16.97
ATOM	3245	N	GLY	B	238	37.041	15.972	45.725	1.00	15.04
ATOM	3246	CA	GLY	B	238	37.550	14.686	46.165	1.00	15.25
ATOM	3247	C	GLY	B	238	36.856	13.544	45.468	1.00	11.48
ATOM	3248	O	GLY	B	238	36.743	12.446	46.018	1.00	10.44
ATOM	3249	N	ILE	B	239	36.376	13.818	44.262	1.00	12.60
ATOM	3250	CA	ILE	B	239	35.681	12.791	43.455	1.00	20.05
ATOM	3251	CB	ILE	B	239	34.728	13.419	42.348	1.00	18.52
ATOM	3252	CG2	ILE	B	239	34.030	12.323	41.541	1.00	15.35
ATOM	3253	CG1	ILE	B	239	33.629	14.264	43.004	1.00	15.89
ATOM	3254	CD1	ILE	B	239	32.833	15.116	42.060	1.00	14.48
ATOM	3255	C	ILE	B	239	36.765	11.933	42.789	1.00	22.58
ATOM	3256	O	ILE	B	239	37.733	12.422	42.182	1.00	24.58
ATOM	3257	N	ALA	B	240	36.618	10.629	42.972	1.00	25.46
ATOM	3258	CA	ALA	B	240	37.549	9.658	42.388	1.00	30.26
ATOM	3259	CB	ALA	B	240	38.709	9.371	43.348	1.00	28.80
ATOM	3260	C	ALA	B	240	36.745	8.387	42.113	1.00	34.31
ATOM	3261	O	ALA	B	240	35.791	8.054	42.807	1.00	37.19
ATOM	3262	N	GLY	B	241	37.092	7.707	41.031	1.00	39.62
ATOM	3263	CA	GLY	B	241	36.391	6.486	40.708	1.00	42.87
ATOM	3264	C	GLY	B	241	36.177	6.350	39.226	1.00	47.59
ATOM	3265	O	GLY	B	241	36.675	7.159	38.430	1.00	50.53
ATOM	3266	N	HIS	B	242	35.419	5.320	38.858	1.00	49.74
ATOM	3267	CA	HIS	B	242	35.116	5.023	37.432	1.00	50.10
ATOM	3268	CB	HIS	B	242	34.946	3.503	37.242	1.00	54.63
ATOM	3269	CG	HIS	B	242	35.399	2.997	35.903	1.00	58.41
ATOM	3270	CD2	HIS	B	242	34.978	1.942	35.161	1.00	60.60
ATOM	3271	ND1	HIS	B	242	36.398	3.606	35.166	1.00	59.16
ATOM	3272	CE1	HIS	B	242	36.569	2.952	34.032	1.00	60.65
ATOM	3273	NE2	HIS	B	242	35.719	1.939	34.003	1.00	61.38
ATOM	3274	C	HIS	B	242	33.841	5.805	37.067	1.00	48.10
ATOM	3275	O	HIS	B	242	32.748	5.257	36.827	1.00	47.23
ATOM	3276	N	THR	B	243	34.011	7.125	37.076	1.00	42.49

Fig. 4LLL

ATOM	3277	CA	THR B 243	32.920	8.055	36.769	1.00	39.40
ATOM	3278	CB	THR B 243	33.208	9.434	37.428	1.00	38.53
ATOM	3279	OG1	THR B 243	34.370	10.023	36.825	1.00	40.09
ATOM	3280	CG2	THR B 243	33.458	9.269	38.932	1.00	32.41
ATOM	3281	C	THR B 243	32.703	8.201	35.220	1.00	38.08
ATOM	3282	O	THR B 243	33.596	7.930	34.405	1.00	41.50
ATOM	3283	N	TYR B 244	31.474	8.561	34.835	1.00	34.19
ATOM	3284	CA	TYR B 244	31.114	8.792	33.403	1.00	28.57
ATOM	3285	CB	TYR B 244	29.607	8.849	33.203	1.00	24.09
ATOM	3286	CG	TYR B 244	28.855	7.610	33.592	1.00	23.03
ATOM	3287	CD1	TYR B 244	28.553	6.623	32.645	1.00	22.91
ATOM	3288	CE1	TYR B 244	27.800	5.500	32.993	1.00	23.73
ATOM	3289	CD2	TYR B 244	28.397	7.446	34.895	1.00	23.90
ATOM	3290	CE2	TYR B 244	27.648	6.350	35.258	1.00	26.28
ATOM	3291	CZ	TYR B 244	27.340	5.381	34.314	1.00	28.03
ATOM	3292	OH	TYR B 244	26.506	4.354	34.713	1.00	29.78
ATOM	3293	C	TYR B 244	31.699	10.155	33.000	1.00	29.97
ATOM	3294	O	TYR B 244	31.805	10.506	31.824	1.00	31.34
ATOM	3295	N	LEU B 245	31.988	10.968	34.017	1.00	30.30
ATOM	3296	CA	LEU B 245	32.541	12.304	33.783	1.00	27.66
ATOM	3297	CB	LEU B 245	32.641	13.083	35.087	1.00	25.66
ATOM	3298	CG	LEU B 245	33.130	14.529	34.979	1.00	25.02
ATOM	3299	CD1	LEU B 245	32.264	15.339	34.026	1.00	19.31
ATOM	3300	CD2	LEU B 245	33.092	15.147	36.363	1.00	28.05
ATOM	3301	C	LEU B 245	33.892	12.117	33.118	1.00	28.22
ATOM	3302	O	LEU B 245	34.834	11.550	33.662	1.00	30.23
ATOM	3303	N	GLN B 246	33.915	12.536	31.861	1.00	31.69
ATOM	3304	CA	GLN B 246	35.091	12.457	30.995	1.00	34.87
ATOM	3305	CB	GLN B 246	34.621	12.506	29.542	1.00	39.92
ATOM	3306	CG	GLN B 246	35.053	11.300	28.699	1.00	48.51
ATOM	3307	CD	GLN B 246	34.428	9.952	29.137	1.00	52.57
ATOM	3308	OE1	GLN B 246	34.027	9.761	30.296	1.00	50.35
ATOM	3309	NE2	GLN B 246	34.369	9.006	28.199	1.00	53.23
ATOM	3310	C	GLN B 246	36.129	13.544	31.274	1.00	35.82
ATOM	3311	O	GLN B 246	36.701	14.126	30.363	1.00	36.69
ATOM	3312	N	ALA B 247	36.371	13.799	32.556	1.00	38.80
ATOM	3313	CA	ALA B 247	37.355	14.823	33.026	1.00	37.44
ATOM	3314	CB	ALA B 247	36.755	16.208	32.963	1.00	29.80
ATOM	3315	C	ALA B 247	37.753	14.489	34.484	1.00	40.26
ATOM	3316	O	ALA B 247	38.713	15.107	35.015	1.00	40.54
ATOM	3317	OT	ALA B 247	37.091	13.596	35.065	1.00	41.41
ATOM	3318	OH2	HOH 301	18.449	35.278	8.129	1.00	19.95
ATOM	3319	OH2	HOH 302	37.818	28.901	5.084	1.00	3.27
ATOM	3320	OH2	HOH 303 (WAT1)	34.674	20.373	6.663	1.00	2.00
ATOM	3321	OH2	HOH 304	46.125	24.346	-0.517	1.00	13.01
ATOM	3322	OH2	HOH 305	41.359	16.832	8.198	1.00	18.56
ATOM	3323	OH2	HOH 306	44.100	17.051	-9.350	1.00	5.18
ATOM	3324	OH2	HOH 307	42.313	21.456	-12.650	1.00	11.94
ATOM	3325	OH2	HOH 308	36.358	23.401	10.644	1.00	2.00
ATOM	3326	OH2	HOH 309	40.912	41.317	1.744	1.00	2.00
ATOM	3327	OH2	HOH 310	43.309	21.298	13.228	1.00	5.80
ATOM	3328	OH2	HOH 311	32.775	26.065	47.247	1.00	14.47

Fig. 4MMM

ATOM	3329	OH2	HOH	312	11.888	31.064	34.277	1.00	25.86
ATOM	3330	OH2	HOH	313	17.048	17.129	18.493	1.00	37.94
ATOM	3331	OH2	HOH	314	24.428	32.396	46.383	1.00	58.79
ATOM	3332	OH2	HOH	315	31.373	23.719	38.933	1.00	2.00
ATOM	3333	OH2	HOH	316	41.066	20.833	3.872	1.00	13.01
ATOM	3334	OH2	HOH	317	46.600	26.549	2.017	1.00	21.57
ATOM	3335	OH2	HOH	318	34.686	36.202	11.099	1.00	14.87
ATOM	3336	OH2	HOH	319	32.258	44.358	9.093	1.00	32.69
ATOM	3337	OH2	HOH	320	39.030	38.810	-0.342	1.00	28.05
ATOM	3338	OH2	HOH	321	29.475	27.753	-9.404	1.00	22.51
ATOM	3339	OH2	HOH	322	7.826	21.059	36.030	1.00	13.85
ATOM	3340	OH2	HOH	323	28.328	10.413	36.904	1.00	30.16
ATOM	3341	OH2	HOH	324	16.240	17.853	20.766	1.00	36.46
ATOM	3342	OH2	HOH	325	42.574	38.857	13.044	1.00	22.19
ATOM	3343	OH2	HOH	326	48.573	15.605	-1.357	1.00	23.01
ATOM	3344	OH2	HOH	327	32.819	14.796	1.418	1.00	16.33
ATOM	3345	OH2	HOH	328	40.175	25.424	46.900	1.00	10.91
ATOM	3346	OH2	HOH	329	15.148	19.561	50.208	1.00	26.50
ATOM	3347	OH2	HOH	330	27.957	26.048	42.339	1.00	12.44
ATOM	3348	OH2	HOH	331	31.360	18.049	44.986	1.00	26.88
ATOM	3349	OH2	HOH	332	28.746	43.379	9.745	1.00	16.49
ATOM	3350	OH2	HOH	333	10.142	9.048	42.214	1.00	39.64
ATOM	3351	OH2	HOH	334	6.398	19.052	47.895	1.00	13.50
ATOM	3352	OH2	HOH	335	28.631	20.733	14.380	1.00	19.89
ATOM	3353	OH2	HOH	336	45.598	19.716	12.124	1.00	30.51
ATOM	3354	OH2	HOH	337	27.454	27.168	33.433	1.00	23.75
ATOM	3355	OH2	HOH	338(WAT2)	34.176	20.162	3.994	1.00	17.52
ATOM	3356	OH2	HOH	339	26.751	26.551	44.715	1.00	20.42
ATOM	3357	OH2	HOH	340	41.339	18.284	0.754	1.00	18.66
ATOM	3358	OH2	HOH	341	44.857	16.855	1.884	1.00	38.33
ATOM	3359	OH2	HOH	342	12.938	20.618	9.465	1.00	33.17
ATOM	3360	OH2	HOH	343	9.295	13.961	31.913	1.00	36.87

Fig. 5A

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for unliganded HSV2 protease.

Residue Atom	X	Y	Z	B
17 ARG CB	11.93	41.78	7.48	23.77
17 ARG C	13.26	39.77	8.31	23.47
17 ARG O	13.71	39.95	9.46	22.93
17 ARG N	10.94	40.20	9.07	24.64
17 ARG CA	11.86	40.32	7.91	23.58
18 ALA N	13.87	39.03	7.38	22.79
18 ALA CA	15.18	38.40	7.54	20.95
18 ALA CB	15.22	37.13	6.74	18.87
18 ALA C	16.41	39.26	7.17	20.78
18 ALA O	16.33	40.18	6.31	22.23
19 VAL N	17.53	39.00	7.86	18.03
19 VAL CA	18.80	39.69	7.58	16.65
19 VAL CB	19.73	39.85	8.85	16.23
19 VAL CG1	21.11	40.36	8.46	15.83
19 VAL CG2	19.13	40.81	9.84	18.15
19 VAL C	19.49	38.71	6.64	15.42
19 VAL O	19.70	37.54	7.01	16.93
20 PRO N	19.71	39.10	5.37	11.17
20 PRO CD	19.26	40.27	4.61	9.27
20 PRO CA	20.38	38.14	4.50	9.38
20 PRO CB	20.23	38.75	3.12	8.45
20 PRO CG	19.07	39.67	3.25	9.42
20 PRO C	21.82	38.19	4.97	10.57
20 PRO O	22.39	39.28	5.19	10.82
21 ILE N	22.37	37.03	5.26	10.67
21 ILE CA	23.72	36.97	5.73	10.40
21 ILE CB	23.80	36.13	7.05	10.18
21 ILE CG2	25.24	35.79	7.37	13.71

Fig. 5B

Residue Atom	X	Y	Z	B
21 ILE CG1	23.20	36.87	8.24	7.05
21 ILE CD1	22.98	35.95	9.42	6.43
21 ILE C	24.42	36.24	4.63	11.21
21 ILE O	23.84	35.35	4.04	11.11
22 TYR N	25.64	36.66	4.33	12.65
22 TYR CA	26.50	36.01	3.34	10.47
22 TYR CB	27.16	37.06	2.49	11.30
22 TYR CG	26.17	37.79	1.65	15.61
22 TYR CD1	25.76	37.27	0.41	18.56
22 TYR CE1	24.80	37.91	-0.37	18.37
22 TYR CD2	25.61	38.98	2.08	13.23
22 TYR CE2	24.65	39.63	1.30	17.16
22 TYR CZ	24.26	39.09	0.09	17.86
22 TYR OH	23.30	39.73	-0.65	22.48
22 TYR C	27.55	35.17	4.08	9.27
22 TYR O	28.02	35.58	5.14	7.45
23 VAL N	27.83	33.96	3.60	8.25
23 VAL CA	28.86	33.09	4.20	8.74
23 VAL CB	28.36	31.69	4.57	8.18
23 VAL CG1	29.09	31.19	5.80	7.22
23 VAL CG2	26.87	31.66	4.66	9.15
23 VAL C	29.90	32.81	3.14	9.69
23 VAL O	29.54	32.52	2.00	11.20
24 ALA N	31.17	32.85	3.51	9.13
24 ALA CA	32.27	32.58	2.58	5.59
24 ALA CB	32.84	33.85	2.06	2.62
24 ALA C	33.35	31.79	3.28	5.65
24 ALA O	33.48	31.81	4.51	2.99
25 GLY N	34.09	31.04	2.49	5.77
25 GLY CA	35.17	30.23	3.02	6.58

Fig. 5C

Residue Atom	X	Y	Z	B
25 GLY C	35.55	29.12	2.07	7.51
25 GLY O	34.90	28.91	1.05	7.61
26 PHE N	36.63	28.41	2.40	7.15
26 PHE CA	37.09	27.28	1.61	7.60
26 PHE CB	38.59	27.05	1.82	7.69
26 PHE CG	39.48	27.94	0.98	10.69
26 PHE CD1	39.75	27.62	-0.33	11.02
26 PHE CD2	39.99	29.13	1.49	9.49
26 PHE CE1	40.50	28.48	-1.12	10.54
26 PHE CE2	40.74	29.99	0.69	7.24
26 PHE CZ	40.98	29.66	-0.61	6.87
26 PHE C	36.32	26.04	2.01	7.99
26 PHE O	36.05	25.84	3.20	7.09
27 LEU N	35.91	25.23	1.03	8.63
27 LEU CA	35.20	23.98	1.32	9.80
27 LEU CB	34.35	23.49	0.15	7.49
27 LEU CG	32.94	24.00	-0.06	7.63
27 LEU CD1	32.31	24.50	1.21	2.13
27 LEU CD2	32.97	25.06	-1.07	9.69
27 LEU C	36.25	22.93	1.61	9.77
27 LEU O	35.93	21.86	2.11	12.13
28 ALA N	37.48	23.24	1.23	9.85
28 ALA CA	38.65	22.39	1.43	9.80
28 ALA CB	38.52	21.12	0.63	8.55
28 ALA C	39.90	23.14	1.01	10.74
28 ALA O	39.85	24.19	0.39	11.52
29 LEU N	41.04	22.64	1.44	12.26
29 LEU CA	42.30	23.22	1.06	12.96
29 LEU CB	43.11	23.72	2.27	12.36
29 LEU CG	42.64	25.03	2.94	10.60

Fig. 5D

Residue Atom	X	Y	Z	B
29 LEU CD1	43.35	25.24	4.24	13.63
29 LEU CD2	42.88	26.20	2.05	8.28
29 LEU C	42.99	22.07	0.34	14.02
29 LEU O	42.90	20.92	0.75	12.85
30 TYR N	43.64	22.40	-0.76	16.21
30 TYR CA	44.30	21.45	-1.60	17.27
30 TYR CB	44.66	22.07	-2.92	15.53
30 TYR CG	43.47	22.22	-3.82	11.82
30 TYR CD1	42.51	21.21	-3.89	7.98
30 TYR CE1	41.42	21.35	-4.70	7.53
30 TYR CD2	43.30	23.36	-4.59	11.67
30 TYR CE2	42.21	23.51	-5.40	10.27
30 TYR CZ	41.29	22.51	-5.45	8.26
30 TYR OH	40.24	22.70	-6.28	11.33
30 TYR C	45.45	20.64	-1.06	19.34
30 TYR O	45.46	19.42	-1.26	23.88
31 ASP N	46.46	21.23	-0.46	18.47
31 ASP CA	47.46	20.31	0.02	22.18
31 ASP CB	48.82	20.49	-0.64	23.48
31 ASP CG	49.12	19.40	-1.64	25.72
31 ASP OD1	49.10	18.21	-1.26	25.53
31 ASP OD2	49.33	19.73	-2.83	31.11
31 ASP C	47.57	20.27	1.50	24.40
31 ASP O	48.56	19.77	2.04	26.77
32 SER N	46.46	20.65	2.13	26.99
32 SER CA	46.27	20.72	3.60	27.07
32 SER CB	44.83	21.14	3.92	25.49
32 SER OG	43.90	20.27	3.27	21.44
32 SER C	46.67	19.50	4.47	25.58
32 SER O	47.21	19.66	5.57	26.01

Fig. 5E

Residue Atom	X	Y	Z	B
33 GLY N	46.42	18.30	3.98	22.89
33 GLY CA	46.81	17.14	4.77	21.93
33 GLY C	45.62	16.37	5.31	21.48
33 GLY O	45.69	15.71	6.35	20.64
34 ASP N	44.51	16.46	4.59	22.42
34 ASP CA	43.29	15.74	4.98	21.94
34 ASP CB	42.09	16.12	4.09	19.38
34 ASP CG	41.52	17.48	4.40	18.22
34 ASP OD1	41.43	18.31	3.48	16.27
34 ASP OD2	41.18	17.71	5.57	19.82
34 ASP C	43.54	14.26	4.80	22.11
34 ASP O	44.53	13.85	4.18	24.20
35 PRO N	42.70	13.44	5.41	21.82
35 PRO CD	41.86	13.79	6.56	24.22
35 PRO CA	42.83	11.99	5.29	22.07
35 PRO CB	41.78	11.50	6.27	22.82
35 PRO CG	41.87	12.52	7.35	24.27
35 PRO C	42.46	11.60	3.85	23.00
35 PRO O	41.77	12.34	3.15	22.94
36 GLY N	42.91	10.41	3.43	23.64
36 GLY CA	42.64	9.93	2.09	23.75
36 GLY C	41.24	10.26	1.64	24.43
36 GLY O	41.03	11.01	0.70	23.27
37 GLU N	40.29	9.73	2.38	27.39
37 GLU CA	38.87	9.94	2.11	29.09
37 GLU CB	38.02	9.32	3.25	32.88
37 GLU CG	36.48	9.58	3.18	36.03
37 GLU CD	35.63	8.54	3.98	37.16
37 GLU OE1	35.51	8.66	5.25	36.25
37 GLU OE2	35.11	7.61	3.30	36.95

Fig. 5F

Residue Atom	X	Y	Z	B
37 GLU C	38.55	11.43	1.94	29.01
37 GLU O	38.15	11.87	0.84	32.05
38 LEU N	38.77	12.21	3.00	25.79
38 LEU CA	38.44	13.62	2.95	22.29
38 LEU CB	38.81	14.28	4.28	21.83
38 LEU CG	37.90	13.88	5.44	22.40
38 LEU CD1	36.48	13.63	4.92	18.69
38 LEU CD2	38.44	12.61	6.10	24.95
38 LEU C	39.06	14.39	1.80	21.48
38 LEU O	38.38	15.13	1.08	19.95
39 ALA N	40.36	14.19	1.67	23.17
39 ALA CA	41.19	14.85	0.67	22.76
39 ALA CB	42.49	14.07	0.52	22.75
39 ALA C	40.50	15.06	-0.69	22.96
39 ALA O	40.01	14.11	-1.32	25.23
40 LEU N	40.50	16.30	-1.17	20.76
40 LEU CA	39.87	16.63	-2.43	17.48
40 LEU CB	38.65	17.52	-2.12	16.13
40 LEU CG	37.44	17.70	-3.04	11.75
40 LEU CD1	36.92	16.41	-3.53	7.63
40 LEU CD2	36.40	18.45	-2.26	12.64
40 LEU C	40.90	17.37	-3.29	16.67
40 LEU O	41.38	18.43	-2.90	19.63
41 ASP N	41.30	16.81	-4.41	15.24
41 ASP CA	42.30	17.48	-5.25	15.78
41 ASP CB	43.22	16.47	-5.88	14.72
41 ASP CG	42.56	15.72	-6.99	15.87
41 ASP OD1	42.85	15.99	-8.18	16.55
41 ASP OD2	41.75	14.85	-6.63	15.87
41 ASP C	41.64	18.36	-6.33	16.91

Fig. 5G

Residue Atom	X	Y	Z	B
41 ASP O	40.43	18.28	-6.55	16.56
42 PRO N	42.44	19.17	-7.06	17.31
42 PRO CD	43.90	19.34	-6.96	15.77
42 PRO CA	41.91	20.05	-8.10	16.95
42 PRO CB	43.12	20.93	-8.44	12.88
42 PRO CG	44.21	20.03	-8.25	14.99
42 PRO C	41.22	19.46	-9.33	17.30
42 PRO O	40.29	20.07	-9.88	17.30
43 ASP N	41.64	18.29	-9.78	18.14
43 ASP CA	40.98	17.71	-10.95	18.82
43 ASP CB	41.89	16.70	-11.63	17.15
43 ASP CG	42.74	17.34	-12.71	15.78
43 ASP OD1	43.04	18.55	-12.65	15.07
43 ASP OD2	43.07	16.64	-13.66	19.23
43 ASP C	39.55	17.19	-10.68	19.69
43 ASP O	38.66	17.27	-11.53	20.59
44 THR N	39.33	16.70	-9.47	18.93
44 THR CA	38.03	16.25	-9.04	16.75
44 THR CB	38.17	15.58	-7.68	19.05
44 THR OG1	39.06	14.46	-7.80	20.07
44 THR CG2	36.83	15.17	-7.11	18.19
44 THR C	37.11	17.46	-8.90	15.66
44 THR O	35.95	17.37	-9.25	17.63
45 VAL N	37.63	18.58	-8.40	14.40
45 VAL CA	36.87	19.82	-8.21	12.95
45 VAL CB	37.65	20.83	-7.32	10.87
45 VAL CG1	37.07	22.23	-7.41	8.51
45 VAL CG2	37.62	20.37	-5.91	9.61
45 VAL C	36.46	20.46	-9.55	14.62
45 VAL O	35.34	20.92	-9.73	15.51

Fig. 5H

Residue Atom	X	Y	Z	B
46 ARG N	37.38	20.45	-10.51	16.51
46 ARG CA	37.15	20.98	-11.85	16.58
46 ARG CB	38.44	20.77	-12.66	20.37
46 ARG CG	38.45	21.26	-14.09	26.06
46 ARG CD	39.37	22.49	-14.20	34.14
46 ARG NE	38.95	23.59	-13.30	38.64
46 ARG CZ	39.39	24.85	-13.38	40.55
46 ARG NH1	38.92	25.76	-12.51	40.97
46 ARG NH2	40.32	25.22	-14.30	41.02
46 ARG C	36.02	20.18	-12.49	14.81
46 ARG O	35.16	20.73	-13.13	13.14
47 ALA N	36.08	18.86	-12.34	15.77
47 ALA CA	35.09	17.92	-12.86	15.83
47 ALA CB	35.49	16.52	-12.52	15.76
47 ALA C	33.69	18.19	-12.32	16.84
47 ALA O	32.74	18.09	-13.06	17.38
48 ALA N	33.56	18.52	-11.04	17.21
48 ALA CA	32.28	18.82	-10.41	17.52
48 ALA CB	32.33	18.41	-8.95	17.33
48 ALA C	31.75	20.26	-10.53	17.33
48 ALA O	30.70	20.57	-10.03	16.52
49 LEU N	32.46	21.14	-11.22	17.96
49 LEU CA	32.00	22.52	-11.33	19.43
49 LEU CB	33.05	23.49	-10.79	18.53
49 LEU CG	33.42	23.38	-9.33	16.94
49 LEU CD1	34.37	24.52	-9.02	14.90
49 LEU CD2	32.17	23.38	-8.46	13.36
49 LEU C	31.70	22.93	-12.76	21.68
49 LEU O	32.52	22.70	-13.65	23.49
50 PRO N	30.56	23.63	-12.99	22.44

Fig. 5I

Residue Atom	X	Y	Z	B
50 PRO CD	30.23	24.24	-14.29	20.44
50 PRO CA	29.58	24.03	-11.97	20.59
50 PRO CB	28.68	24.98	-12.73	20.21
50 PRO CG	28.79	24.47	-14.15	20.99
50 PRO C	28.82	22.83	-11.46	20.00
50 PRO O	28.61	21.86	-12.20	19.97
51 PRO N	28.41	22.86	-10.18	18.40
51 PRO CD	28.46	23.88	-9.13	17.89
51 PRO CA	27.67	21.69	-9.71	18.78
51 PRO CB	27.52	21.96	-8.23	16.82
51 PRO CG	27.42	23.42	-8.19	16.19
51 PRO C	26.34	21.57	-10.46	21.71
51 PRO O	25.66	22.57	-10.79	21.62
52 GLU N	26.03	20.32	-10.82	22.45
52 GLU CA	24.83	19.97	-11.54	22.76
52 GLU CB	24.59	18.48	-11.36	24.61
52 GLU CG	23.33	18.02	-11.96	27.88
52 GLU CD	23.50	17.70	-13.40	28.89
52 GLU OE1	23.96	18.61	-14.17	31.44
52 GLU OE2	23.20	16.53	-13.72	26.97
52 GLU C	23.59	20.73	-11.05	22.81
52 GLU O	22.91	21.41	-11.83	23.60
53 ASN N	23.30	20.58	-9.77	20.97
53 ASN CA	22.16	21.23	-9.18	20.23
53 ASN CB	21.16	20.19	-8.71	23.40
53 ASN CG	20.72	19.28	-9.82	28.64
53 ASN OD1	21.10	18.10	-9.84	35.51
53 ASN ND2	19.96	19.81	-10.78	28.10
53 ASN C	22.60	22.05	-8.01	19.30
53 ASN O	23.48	21.64	-7.27	21.50

Fig. 5J

Residue Atom	X	Y	Z	B
54 PRO N	21.94	23.19	-7.77	18.19
54 PRO CD	20.70	23.57	-8.46	19.95
54 PRO CA	22.20	24.13	-6.68	16.41
54 PRO CB	20.89	24.88	-6.54	18.57
54 PRO CG	19.87	23.98	-7.31	19.87
54 PRO C	22.59	23.46	-5.39	13.92
54 PRO O	22.23	22.33	-5.12	11.63
55 LEU N	23.35	24.17	-4.59	13.45
55 LEU CA	23.81	23.57	-3.37	12.25
55 LEU CB	25.33	23.72	-3.26	15.69
55 LEU CG	26.14	22.73	-4.07	14.38
55 LEU CD1	27.55	23.24	-4.23	15.31
55 LEU CD2	26.12	21.42	-3.31	17.14
55 LEU C	23.13	24.14	-2.16	10.90
55 LEU O	23.34	25.31	-1.83	14.26
56 PRO N	22.28	23.34	-1.50	8.09
56 PRO CD	21.86	21.96	-1.78	8.27
56 PRO CA	21.62	23.86	-0.31	7.83
56 PRO CB	20.55	22.82	-0.05	6.41
56 PRO CG	21.21	21.55	-0.50	5.90
56 PRO C	22.58	23.95	0.87	8.56
56 PRO O	23.55	23.20	0.98	6.85
57 ILE N	22.33	24.95	1.70	8.07
57 ILE CA	23.11	25.14	2.90	6.88
57 ILE CB	23.57	26.60	3.08	3.62
57 ILE CG2	24.46	26.72	4.32	3.19
57 ILE CG1	24.31	27.07	1.84	2.00
57 ILE CD1	24.90	28.39	1.99	2.00
57 ILE C	22.15	24.77	4.04	7.47
57 ILE O	21.08	25.36	4.19	8.61

Fig. 5K

Residue Atom	X	Y	Z	B
58 ASN N	22.47	23.71	4.77	5.54
58 ASN CA	21.63	23.31	5.87	6.46
58 ASN CB	21.03	21.94	5.61	4.75
58 ASN CG	22.05	20.93	5.24	6.39
58 ASN OD1	23.08	20.84	5.87	6.72
58 ASN ND2	21.75	20.14	4.23	6.81
58 ASN C	22.44	23.32	7.18	8.53
58 ASN O	23.65	23.56	7.16	10.73
59 VAL N	21.78	23.13	8.32	5.59
59 VAL CA	22.48	23.13	9.58	3.21
59 VAL CB	21.70	23.87	10.69	2.76
59 VAL CG1	22.40	23.70	12.01	2.00
59 VAL CG2	21.61	25.35	10.37	2.00
59 VAL C	22.85	21.74	10.03	4.47
59 VAL O	22.02	20.86	10.09	4.87
60 ASP N	24.14	21.54	10.22	6.21
60 ASP CA	24.72	20.29	10.69	9.27
60 ASP CB	24.50	20.16	12.22	12.92
60 ASP CG	25.64	19.40	12.93	18.52
60 ASP OD1	26.78	19.39	12.40	23.62
60 ASP OD2	25.43	18.84	14.04	15.83
60 ASP C	24.21	19.05	9.96	10.71
60 ASP O	23.88	18.06	10.57	12.47
61 HIS N	24.13	19.11	8.64	12.79
61 HIS CA	23.68	17.98	7.81	14.32
61 HIS C	22.24	17.54	7.92	17.79
61 HIS O	21.85	16.59	7.25	20.60
61 HIS CB	24.59	16.76	7.96	10.25
61 HIS CG	26.00	17.01	7.52	12.30
61 HIS ND1	26.39	17.08	6.21	13.19

Fig. 5L

Residue Atom	X	Y	Z	B
61 HIS CD2	27.10	17.30	8.26	11.24
61 HIS NE2	28.16	17.57	7.41	13.47
61 HIS CE1	27.69	17.42	6.18	11.79
62 ARG N	21.44	18.20	8.76	18.10
62 ARG CA	20.03	17.86	8.88	17.04
62 ARG CB	19.45	18.45	10.16	21.61
62 ARG CG	18.73	17.42	11.06	28.55
62 ARG CD	17.22	17.21	10.64	35.65
62 ARG NE	16.32	18.30	11.07	37.04
62 ARG CZ	15.69	18.35	12.26	39.49
62 ARG NH1	15.85	17.36	13.16	37.41
62 ARG NH2	14.86	19.36	12.53	39.13
62 ARG C	19.32	18.45	7.68	15.19
62 ARG O	19.09	19.65	7.62	16.59
63 ALA N	19.06	17.61	6.69	14.69
63 ALA CA	18.39	18.02	5.45	16.12
63 ALA CB	18.05	16.81	4.61	14.80
63 ALA C	17.14	18.86	5.74	17.87
63 ALA O	16.92	19.85	5.05	19.17
64 ARG N	16.37	18.50	6.78	20.11
64 ARG CA	15.16	19.26	7.18	20.31
64 ARG CB	14.38	18.58	8.30	23.48
64 ARG CG	13.07	19.33	8.64	26.43
64 ARG CD	12.35	18.73	9.83	28.44
64 ARG NE	12.20	17.28	9.69	29.46
64 ARG CZ	12.46	16.41	10.66	32.40
64 ARG NH1	12.88	16.85	11.85	34.22
64 ARG NH2	12.25	15.10	10.46	32.33
64 ARG C	15.40	20.73	7.59	18.85
64 ARG O	14.45	21.52	7.53	19.05

Fig. 5M

Residue Atom	X	Y	Z	B
65 CYS N	16.61	21.06	8.10	16.40
65 CYS CA	16.93	22.44	8.46	14.24
65 CYS CB	17.78	22.57	9.72	11.24
65 CYS SG	17.17	21.76	11.09	19.10
65 CYS C	17.77	22.99	7.36	13.25
65 CYS O	18.96	22.93	7.45	17.07
66 GLU N	17.15	23.47	6.30	9.68
66 GLU CA	17.89	24.05	5.23	8.49
66 GLU CB	17.27	23.62	3.93	7.02
66 GLU CG	17.73	24.38	2.73	9.23
66 GLU CD	17.32	23.71	1.45	10.47
66 GLU OE1	17.44	22.48	1.36	11.03
66 GLU OE2	16.89	24.43	0.53	10.11
66 GLU C	17.66	25.50	5.47	9.58
66 GLU O	16.54	25.87	5.61	13.45
67 VAL N	18.71	26.31	5.54	9.57
67 VAL CA	18.57	27.74	5.81	5.68
67 VAL CB	19.30	28.16	7.10	8.71
67 VAL CG1	18.71	27.45	8.32	7.38
67 VAL CG2	20.81	27.87	6.98	5.47
67 VAL C	19.09	28.61	4.69	5.54
67 VAL O	19.09	29.82	4.82	4.42
68 GLY N	19.51	28.00	3.59	6.23
68 GLY CA	20.02	28.80	2.48	7.33
68 GLY C	20.49	28.11	1.22	9.75
68 GLY O	20.25	26.92	1.01	11.38
69 ARG N	21.25	28.85	0.43	9.67
69 ARG CA	21.73	28.37	-0.85	9.65
69 ARG CB	20.75	28.95	-1.89	13.32
69 ARG CG	21.10	28.85	-3.38	17.79

Fig. 5N

Résidue Atom	X	Y	Z	B
69 ARG CD	21.07	27.45	-3.86	20.10
69 ARG NE	20.21	26.67	-2.99	25.53
69 ARG CZ	18.90	26.54	-3.13	28.17
69 ARG NH1	18.23	25.78	-2.23	29.80
69 ARG NH2	18.26	27.11	-4.16	26.46
69 ARG C	23.17	28.82	-1.13	8.83
69 ARG O	23.56	29.93	-0.74	10.07
70 VAL N	23.96	27.98	-1.79	6.16
70 VAL CA	25.31	28.36	-2.17	5.74
70 VAL CB	26.17	27.13	-2.48	3.22
70 VAL CG1	27.46	27.51	-3.18	2.00
70 VAL CG2	26.49	26.43	-1.23	2.00
70 VAL C	25.20	29.22	-3.45	7.31
70 VAL O	24.71	28.73	-4.46	9.38
71 LEU N	25.57	30.50	-3.40	7.30
71 LEU CA	25.54	31.38	-4.58	7.19
71 LEU CB	25.67	32.83	-4.15	5.22
71 LEU CG	24.62	33.30	-3.17	5.66
71 LEU CD1	24.80	34.76	-2.88	2.00
71 LEU CD2	23.25	33.04	-3.76	10.02
71 LEU C	26.57	31.04	-5.71	9.63
71 LEU O	26.20	30.98	-6.89	11.03
72 ALA N	27.84	30.82	-5.36	9.00
72 ALA CA	28.89	30.46	-6.30	7.85
72 ALA CB	29.54	31.68	-6.80	9.83
72 ALA C	29.95	29.57	-5.63	9.95
72 ALA O	30.10	29.58	-4.41	11.10
73 VAL N	30.62	28.74	-6.42	11.11
73 VAL CA	31.71	27.87	-5.93	12.90
73 VAL CB	31.37	26.34	-5.96	12.82

Fig. 50

Residue Atom	X	Y	Z	B
73 VAL CG1	32.48	25.51	-5.30	10.03
73 VAL CG2	30.06	26.07	-5.26	14.65
73 VAL C	32.78	28.16	-6.97	13.82
73 VAL O	32.48	28.19	-8.15	15.35
74 VAL N	34.00	28.47	-6.53	13.95
74 VAL CA	35.07	28.80	-7.46	15.06
74 VAL CB	35.41	30.29	-7.33	15.62
74 VAL CG1	36.72	30.58	-8.04	18.50
74 VAL CG2	34.31	31.14	-7.90	13.45
74 VAL C	36.31	28.00	-7.14	15.92
74 VAL O	36.66	27.87	-5.97	18.48
75 ASN N	36.98	27.46	-8.15	15.92
75 ASN CA	38.22	26.71	-7.89	15.66
75 ASN CB	38.46	25.68	-9.00	16.57
75 ASN CG	39.67	24.82	-8.74	18.18
75 ASN OD1	40.18	24.16	-9.63	20.99
75 ASN ND2	40.12	24.81	-7.52	20.52
75 ASN C	39.41	27.67	-7.77	14.23
75 ASN O	39.91	28.19	-8.75	16.41
76 ASP N	39.79	27.99	-6.56	13.61
76 ASP CA	40.91	28.87	-6.33	13.15
76 ASP CB	40.66	29.63	-5.04	15.03
76 ASP CG	41.88	30.35	-4.50	15.79
76 ASP OD1	42.60	29.74	-3.69	17.48
76 ASP OD2	42.11	31.54	-4.82	13.72
76 ASP C	42.14	27.95	-6.24	13.28
76 ASP O	42.02	26.80	-5.83	15.73
77 PRO N	43.32	28.43	-6.62	10.71
77 PRO CD	43.67	29.79	-7.06	9.86

Fig. 5P

Residue Atom	X	Y	Z	B
77 PRO CA	44.52	27.60	-6.56	10.08
77 PRO CB	45.61	28.61	-6.79	8.87
77 PRO CG	44.98	29.58	-7.67	7.64
77 PRO C	44.70	26.87	-5.22	11.39
77 PRO O	45.34	25.83	-5.16	10.85
78 ARG N	44.11	27.43	-4.16	10.81
78 ARG CA	44.20	26.85	-2.83	11.79
78 ARG CB	44.22	27.95	-1.78	10.22
78 ARG CG	45.36	28.94	-1.94	12.52
78 ARG CD	45.44	29.88	-0.75	16.01
78 ARG NE	45.45	29.10	0.51	22.19
78 ARG CZ	45.12	29.57	1.72	21.40
78 ARG NH1	45.17	28.76	2.77	21.39
78 ARG NH2	44.75	30.83	1.92	21.43
78 ARG C	43.10	25.83	-2.52	12.63
78 ARG O	43.29	24.93	-1.69	12.90
79 GLY N	41.95	25.95	-3.18	11.40
79 GLY CA	40.85	25.04	-2.95	9.61
79 GLY C	39.57	25.69	-3.39	8.97
79 GLY O	39.60	26.87	-3.76	8.84
80 PRO N	38.44	24.95	-3.41	8.44
80 PRO CD	38.32	23.52	-3.09	9.93
80 PRO CA	37.13	25.49	-3.82	8.23
80 PRO CB	36.28	24.23	-3.91	7.99
80 PRO CG	36.85	23.35	-2.92	8.18
80 PRO C	36.63	26.47	-2.77	8.23
80 PRO O	36.51	26.15	-1.60	10.20
81 PHE N	36.49	27.71	-3.17	7.10
81 PHE CA	36.03	28.73	-2.26	9.63
81 PHE CB	36.87	29.98	-2.47	8.78

Fig. 5Q

Residue Atom	X	Y	Z	B
81 PHE CG	36.40	31.19	-1.70	11.26
81 PHE CD1	36.84	31.42	-0.40	6.17
81 PHE CD2	35.53	32.14	-2.29	11.51
81 PHE CE1	36.45	32.56	0.29	6.96
81 PHE CE2	35.13	33.28	-1.59	8.50
81 PHE CZ	35.60	33.49	-0.30	7.53
81 PHE C	34.57	28.97	-2.63	13.60
81 PHE O	34.24	29.13	-3.82	15.81
82 PHE N	33.67	28.96	-1.64	13.48
82 PHE CA	32.26	29.18	-1.91	12.13
82 PHE CB	31.42	27.98	-1.46	8.73
82 PHE CG	30.82	28.12	-0.12	7.25
82 PHE CD1	29.47	28.33	0.02	8.88
82 PHE CD2	31.61	28.07	1.01	8.28
82 PHE CE1	28.91	28.48	1.27	8.50
82 PHE CE2	31.04	28.22	2.27	6.88
82 PHE CZ	29.70	28.43	2.40	4.53
82 PHE C	31.75	30.45	-1.23	12.39
82 PHE O	32.44	31.07	-0.42	16.47
83 VAL N	30.55	30.86	-1.62	9.90
83 VAL CA	29.89	32.01	-1.04	11.13
83 VAL CB	30.03	33.25	-1.92	9.41
83 VAL CG1	29.04	34.31	-1.48	6.73
83 VAL CG2	31.44	33.81	-1.82	12.28
83 VAL C	28.43	31.62	-0.97	12.70
83 VAL O	27.87	31.20	-1.97	13.65
84 GLY N	27.81	31.72	0.21	10.38
84 GLY CA	26.41	31.35	0.33	8.03
84 GLY C	25.57	32.42	0.94	6.01

Fig. 5R

Residue Atom	X	Y	Z	B
84 GLY O	26.07	33.37	1.52	6.85
85 LEU N	24.27	32.29	0.78	5.76
85 LEU CA	23.30	33.23	1.34	8.07
85 LEU CB	22.43	33.82	0.24	7.19
85 LEU CG	21.35	34.78	0.70	7.85
85 LEU CD1	21.89	36.19	0.89	6.18
85 LEU CD2	20.24	34.76	-0.35	11.21
85 LEU C	22.40	32.54	2.37	8.00
85 LEU O	21.99	31.41	2.19	6.96
86 ILE N	22.10	33.23	3.46	8.19
86 ILE CA	21.27	32.66	4.50	7.74
86 ILE CB	22.11	32.40	5.73	8.25
86 ILE CG2	21.26	31.83	6.81	6.69
86 ILE CG1	23.30	31.51	5.37	2.00
86 ILE CD1	24.13	31.13	6.56	4.98
86 ILE C	20.15	33.62	4.85	8.36
86 ILE O	20.39	34.64	5.47	12.27
87 ALA N	18.94	33.36	4.37	8.37
87 ALA CA	17.80	34.23	4.67	9.29
87 ALA CB	17.16	34.76	3.39	5.71
87 ALA C	16.82	33.39	5.46	8.92
87 ALA O	16.08	32.59	4.89	9.22
88 CYS N	16.84	33.55	6.77	8.19
88 CYS CA	16.01	32.74	7.65	9.16
88 CYS CB	16.71	31.40	7.88	6.92
88 CYS SG	15.87	30.13	8.78	5.83
88 CYS C	15.89	33.51	8.95	11.52
88 CYS O	16.88	33.64	9.67	14.84
89 VAL N	14.72	34.05	9.25	13.03
89 VAL CA	14.52	34.79	10.48	11.73

Fig. 5S

Residue Atom	X	Y	Z	B
89 VAL CB	13.45	35.90	10.31	13.04
89 VAL CG1	12.07	35.28	10.12	15.08
89 VAL CG2	13.49	36.86	11.49	12.47
89 VAL C	14.26	33.88	11.68	11.56
89 VAL O	14.28	34.33	12.81	10.96
90 GLN N	14.04	32.59	11.43	11.77
90 GLN CA	13.85	31.61	12.51	12.33
90 GLN CB	13.14	30.36	12.03	10.30
90 GLN CG	11.67	30.55	11.89	13.90
90 GLN CD	11.00	29.31	11.36	17.26
90 GLN OE1	11.68	28.34	11.01	17.86
90 GLN NE2	9.67	29.31	11.31	14.90
90 GLN C	15.20	31.25	13.12	13.24
90 GLN O	15.34	31.18	14.33	14.62
91 LEU N	16.20	31.01	12.28	12.44
91 LEU CA	17.56	30.72	12.74	11.11
91 LEU CB	18.45	30.49	11.54	9.40
91 LEU CG	19.93	30.33	11.76	8.68
91 LEU CD1	20.18	29.11	12.58	9.22
91 LEU CD2	20.61	30.19	10.45	9.24
91 LEU C	18.01	31.98	13.47	11.99
91 LEU O	18.61	31.92	14.53	11.04
92 GLU N	17.66	33.11	12.91	12.25
92 GLU CA	18.02	34.37	13.51	14.20
92 GLU CB	17.63	35.50	12.56	19.07
92 GLU CG	17.52	36.89	13.19	21.54
92 GLU CD	16.97	37.88	12.19	23.75
92 GLU OE1	17.21	37.67	10.96	19.07
92 GLU OE2	16.29	38.85	12.66	24.68
92 GLU C	17.44	34.58	14.89	13.85

Fig. 5T

Residue Atom	X	Y	Z	B
92 GLU O	18.16	35.01	15.79	16.48
93 ARG N	16.16	34.28	15.09	13.91
93 ARG CA	15.51	34.47	16.39	11.99
93 ARG CB	13.98	34.51	16.24	15.54
93 ARG CG	13.44	35.55	15.26	20.43
93 ARG CD	13.70	37.04	15.62	27.76
93 ARG NE	13.09	37.90	14.59	33.37
93 ARG CZ	13.19	39.24	14.47	32.48
93 ARG NH1	12.56	39.85	13.46	34.48
93 ARG NH2	13.90	39.98	15.32	31.73
93 ARG C	15.89	33.42	17.45	9.12
93 ARG O	16.18	33.77	18.59	9.17
94 VAL N	15.89	32.16	17.05	6.89
94 VAL CA	16.24	31.05	17.93	.02
94 VAL CB	16.48	29.77	17.13	5.90
94 VAL CG1	17.00	28.67	18.01	5.97
94 VAL CG2	15.22	29.34	16.50	10.65
94 VAL C	17.52	31.37	18.68	10.18
94 VAL O	17.59	31.16	19.90	11.82
95 LEU N	18.53	31.85	17.95	10.80
95 LEU CA	19.83	32.21	18.50	10.14
95 LEU CB	20.81	32.54	17.36	9.46
95 LEU CG	21.99	31.63	16.98	8.46
95 LEU CD1	21.83	30.26	17.59	8.92
95 LEU CD2	22.12	31.55	15.46	2.00
95 LEU C	19.66	33.41	19.42	11.97
95 LEU O	20.00	33.32	20.60	11.21
96 GLU N	19.11	34.52	18.91	14.36
96 GLU CA	18.92	35.74	19.71	16.50
96 GLU CB	18.11	36.80	18.97	18.80

Fig. 5U

Residue Atom	X	Y	Z	B
96 GLU CG	18.81	37.50	17.84	23.30
96 GLU CD	17.84	38.28	16.98	29.76
96 GLU OE1	18.33	39.02	16.07	32.86
96 GLU OE2	16.59	38.15	17.20	28.34
96 GLU C	18.22	35.49	21.03	16.75
96 GLU O	18.39	36.21	22.01	15.67
97 THR N	17.33	34.54	21.03	16.21
97 THR CA	16.68	34.27	22.27	19.53
97 THR CB	15.25	33.77	22.05	21.08
97 THR OG1	15.26	32.62	21.20	21.77
97 THR CG2	14.43	34.84	21.37	22.70
97 THR C	17.54	33.32	23.13	19.94
97 THR O	17.75	33.57	24.32	22.37
98 ALA N	18.09	32.27	22.50	18.83
98 ALA CA	18.91	31.28	23.19	14.28
98 ALA CB	19.60	30.40	22.19	13.42
98 ALA C	19.93	31.98	24.01	13.36
98 ALA O	20.08	31.72	25.19	14.87
99 ALA N	20.60	32.94	23.40	13.17
99 ALA CA	21.63	33.69	24.08	15.11
99 ALA CB	22.40	34.60	23.12	12.19
99 ALA C	20.97	34.51	25.10	18.62
99 ALA O	20.46	35.59	24.80	21.12
100 SER N	20.95	33.99	26.33	22.85
100 SER CA	20.41	34.73	27.48	26.09
100 SER CB	20.05	33.73	28.59	24.21
100 SER OG	19.10	32.79	28.11	22.05
100 SER C	21.66	35.63	27.83	26.19
100 SER O	22.04	35.88	29.00	23.67
101 ALA N	22.20	36.16	26.75	25.61

Fig. 5V

Residue Atom	X	Y	Z	B
101 ALA CA	23.37	36.94	26.73	28.22
101 ALA CB	23.54	37.60	25.37	28.74
101 ALA C	23.49	37.96	27.81	29.83
101 ALA O	22.76	38.98	27.82	30.02
102 ALA N	24.35	37.61	28.77	30.00
102 ALA CA	24.70	38.56	29.82	30.27
102 ALA CB	25.58	37.91	30.86	31.28
102 ALA C	25.57	39.33	28.83	29.14
102 ALA O	25.24	40.43	28.39	28.35
103 ILE N	26.44	38.53	28.25	29.66
103 ILE CA	27.37	38.98	27.25	33.49
103 ILE CB	28.76	39.19	27.89	33.70
103 ILE C	27.41	37.85	26.21	35.49
103 ILE O	28.33	37.87	25.33	36.26
103 ILE OT	26.56	36.91	26.34	36.09
113 ARG CB	23.51	46.04	17.34	18.99
113 ARG CG	24.59	47.13	17.30	20.59
113 ARG CD	25.59	47.03	18.47	25.46
113 ARG NE	26.33	45.76	18.47	29.74
113 ARG CZ	26.69	45.09	19.57	28.63
113 ARG NH1	27.36	43.93	19.47	26.03
113 ARG NH2	26.40	45.60	20.77	31.45
113 ARG C	22.24	44.52	15.77	20.25
113 ARG O	21.47	43.97	16.52	21.30
113 ARG N	21.85	47.03	15.77	22.12
113 ARG CA	22.77	45.91	16.00	19.32
114 GLU N	22.59	44.05	14.60	23.15
114 GLU CA	22.34	42.73	14.04	23.09
114 GLU CB	21.77	42.92	12.65	24.43
114 GLU CG	22.55	43.98	11.90	27.32
114 GLU CD	22.26	43.99	10.42	33.37

Fig. 5W

Residue Atom	X	Y	Z	B
114 GLU OE1	21.80	42.94	9.89	35.72
114 GLU OE2	22.51	45.06	9.79	34.77
114 GLU C	23.79	42.18	13.92	22.64
114 GLU O	24.08	41.27	13.15	20.26
115 GLU N	24.69	42.89	14.60	22.39
115 GLU CA	26.10	42.60	14.73	20.62
115 GLU CB	26.85	43.88	15.18	22.97
115 GLU CG	27.12	44.94	14.04	31.25
115 GLU CD	25.99	46.01	13.77	37.09
115 GLU OE1	25.17	46.29	14.68	38.27
115 GLU OE2	25.93	46.60	12.64	36.47
115 GLU C	26.07	41.52	15.82	18.19
115 GLU O	26.87	40.61	15.84	16.89
116 ARG N	25.06	41.59	16.67	18.07
116 ARG CA	24.84	40.62	17.73	17.02
116 ARG CB	23.68	41.05	18.62	19.38
116 ARG CG	24.02	41.10	20.15	29.57
116 ARG CD	24.12	39.70	20.92	30.71
116 ARG NE	24.52	39.92	22.32	32.10
116 ARG CZ	25.77	39.76	22.78	33.92
116 ARG NH1	26.73	39.34	21.95	33.08
116 ARG NH2	26.07	40.15	24.04	33.45
116 ARG C	24.49	39.31	17.06	14.36
116 ARG O	24.93	38.27	17.50	15.85
117 LEU N	23.67	39.39	16.02	12.55
117 LEU CA	23.27	38.20	15.27	11.60
117 LEU CB	22.25	38.55	14.17	10.36
117 LEU CG	21.97	37.39	13.20	11.78
117 LEU CD1	21.28	36.26	13.94	10.40
117 LEU CD2	21.18	37.83	11.95	9.62

Fig. 5X

Residue Atom	X	Y	Z	B
117 LEU C	24.51	37.57	14.63	12.59
117 LEU O	24.73	36.35	14.74	14.14
118 LEU N	25.32	38.40	13.97	10.04
118 LEU CA	26.52	37.92	13.34	8.44
118 LEU CB	27.17	39.06	12.59	6.10
118 LEU CG	26.92	39.21	11.11	4.04
118 LEU CD1	26.22	38.02	10.54	2.00
118 LEU CD2	26.22	40.51	10.86	2.00
118 LEU C	27.52	37.32	14.33	9.99
118 LEU O	28.18	36.33	14.04	11.91
119 TYR N	27.59	37.90	15.52	11.11
119 TYR CA	28.49	37.42	16.56	12.87
119 TYR CB	28.61	38.46	17.68	17.73
119 TYR CG	29.24	38.00	18.98	22.08
119 TYR CD1	28.54	37.18	19.87	24.95
119 TYR CE1	29.06	36.83	21.09	25.82
119 TYR CD2	30.50	38.46	19.36	22.55
119 TYR CE2	31.03	38.12	20.57	24.18
119 TYR CZ	30.30	37.31	21.43	27.76
119 TYR OH	30.77	37.00	22.69	36.13
119 TYR C	28.04	36.06	17.09	12.48
119 TYR O	28.88	35.20	17.37	14.79
120 LEU N	26.73	35.85	17.18	9.50
120 LEU CA	26.20	34.60	17.66	6.08
120 LEU CB	24.73	34.78	18.06	6.24
120 LEU CG	24.30	35.27	19.45	5.20
120 LEU CD1	24.96	36.55	19.82	6.12
120 LEU CD2	22.83	35.47	19.46	4.68
120 LEU C	26.36	33.45	16.66	4.31
120 LEU O	26.77	32.35	17.01	3.72

Fig. 5Y

Residue Atom	X	Y	Z	B
121 ILE N	26.06	33.73	15.39	2.53
121 ILE CA	26.16	32.69	14.37	3.35
121 ILE CB	25.36	33.09	13.09	3.10
121 ILE CG2	25.98	34.28	12.42	3.81
121 ILE CG1	25.33	31.95	12.07	3.74
121 ILE CD1	24.37	30.88	12.38	8.68
121 ILE C	27.60	32.30	14.04	5.31
121 ILE O	27.89	31.12	13.86	5.15
122 THR N	28.52	33.28	14.05	5.85
122 THR CA	29.94	33.03	13.76	4.14
122 THR CB	30.72	34.30	13.73	3.64
122 THR OG1	30.31	35.09	12.62	7.50
122 THR CG2	32.19	33.99	13.61	2.50
122 THR C	30.64	32.10	14.72	5.58
122 THR O	31.31	31.16	14.31	5.86
123 ASN N	30.50	32.38	16.02	7.95
123 ASN CA	31.11	31.58	17.08	7.96
123 ASN CB	31.24	32.40	18.35	9.01
123 ASN CG	32.26	33.52	18.22	10.01
123 ASN OD1	31.93	34.70	18.14	6.01
123 ASN ND2	33.52	33.13	18.16	12.74
123 ASN C	30.40	30.27	17.34	8.91
123 ASN O	31.02	29.31	17.77	12.08
124 TYR N	29.10	30.21	17.07	9.22
124 TYR CA	28.35	28.97	17.27	9.33
124 TYR CB	26.83	29.25	17.42	6.09
124 TYR CG	26.10	28.12	18.13	2.89
124 TYR CD1	26.21	27.98	19.51	2.00
124 TYR CE1	25.65	26.90	20.16	2.00
124 TYR CD2	25.41	27.15	17.43	2.96

Fig. 52

Residue Atom	X	Y	Z	B
124 TYR CE2	24.85	26.06	18.08	2.00
124 TYR CZ	24.98	25.95	19.44	2.00
124 TYR OH	24.45	24.90	20.09	8.86
124 TYR C	28.65	27.97	16.13	8.61
124 TYR O	28.92	26.79	16.35	8.04
125 LEU N	28.61	28.45	14.91	9.47
125 LEU CA	28.87	27.57	13.78	10.58
125 LEU CB	27.57	27.34	13.02	12.80
125 LEU CG	26.38	26.77	13.80	8.87
125 LEU CD1	25.14	27.30	13.12	10.24
125 LEU CD2	26.40	25.25	13.86	6.51
125 LEU C	29.96	28.21	12.90	10.55
125 LEU O	29.67	28.87	11.88	7.34
126 PRO N	31.23	28.02	13.29	11.29
126 PRO CD	31.71	27.28	14.47	10.63
126 PRO CA	32.37	28.57	12.56	9.46
126 PRO CB	33.49	28.56	13.60	7.45
126 PRO CG	32.85	28.11	14.89	8.18
126 PRO C	32.81	27.76	11.35	9.95
126 PRO O	33.57	28.28	10.53	10.59
127 SER N	32.35	26.51	11.23	7.34
127 SER CA	32.78	25.64	10.14	7.69
127 SER CB	33.33	24.36	10.71	7.69
127 SER OG	34.45	24.61	11.53	12.66
127 SER C	31.75	25.27	9.10	7.85
127 SER O	30.58	25.48	9.30	11.85
128 VAL N	32.23	24.80	7.95	4.94
128 VAL CA	31.36	24.32	6.89	5.12
128 VAL CB	31.40	25.12	5.59	2.60
128 VAL CG1	31.07	26.50	5.86	11.40

Fig. 5AA

Residue Atom	X	Y	Z	B
128 VAL CG2	32.70	25.03	4.93	2.00
128 VAL C	31.84	22.93	6.62	7.19
128 VAL O	32.97	22.58	6.92	11.48
129 SER N	30.97	22.13	6.04	6.97
129 SER CA	31.32	20.78	5.73	7.38
129 SER CB	30.73	19.90	6.80	8.32
129 SER OG	31.11	18.56	6.62	14.12
129 SER C	30.68	20.52	4.37	9.06
129 SER O	29.51	20.77	4.20	11.11
130 LEU N	31.47	20.13	3.38	8.54
130 LEU CA	30.93	19.85	2.07	8.69
130 LEU CB	31.97	20.16	0.99	12.13
130 LEU CG	31.88	19.67	-0.47	11.59
130 LEU CD1	30.63	20.19	-1.18	7.88
130 LEU CD2	33.15	20.15	-1.20	12.99
130 LEU C	30.56	18.41	1.96	7.67
130 LEU O	31.36	17.56	2.22	10.85
131 SER N	29.32	18.10	1.66	7.41
131 SER CA	29.03	16.71	1.46	10.24
131 SER CB	27.65	16.35	1.96	12.02
131 SER OG	27.68	16.30	3.36	18.85
131 SER C	29.16	16.49	-0.04	12.33
131 SER O	28.84	17.37	-0.85	13.24
132 THR N	29.73	15.36	-0.41	14.15
132 THR CA	29.89	14.98	-1.80	15.87
132 THR CB	31.34	14.59	-2.10	13.37
132 THR OG1	31.80	13.73	-1.08	12.74
132 THR CG2	32.24	15.82	-2.18	11.44
132 THR C	29.00	13.77	-1.94	18.29
132 THR O	29.23	12.74	-1.28	19.88

Fig. 5BB

Residue Atom	X	Y	Z	B
133 LYS N	27.94	13.93	-2.72	22.98
133 LYS CA	26.95	12.87	-2.99	26.56
133 LYS CB	25.72	13.45	-3.76	22.20
133 LYS C	27.51	11.62	-3.73	27.59
133 LYS O	28.76	11.46	-3.88	23.36
133 LYS OT	26.63	10.80	-4.13	33.47
141 PRO CB	35.57	12.86	-10.86	23.68
141 PRO C	33.22	13.47	-11.76	26.20
141 PRO O	33.51	13.12	-12.90	24.99
141 PRO N	33.44	11.63	-10.15	31.18
141 PRO CA	34.01	12.96	-10.54	28.79
142 ASP N	32.12	14.16	-11.45	25.77
142 ASP CA	31.21	14.78	-12.41	24.78
142 ASP CB	30.18	13.81	-13.02	22.65
142 ASP CG	29.62	12.83	-12.03	20.99
142 ASP OD1	29.84	12.97	-10.82	22.51
142 ASP OD2	28.98	11.87	-12.49	19.92
142 ASP C	30.52	15.89	-11.63	24.33
142 ASP O	30.73	16.00	-10.43	24.66
143 ARG N	29.65	16.66	-12.28	23.24
143 ARG CA	29.00	17.79	-11.63	22.71
143 ARG CB	28.28	18.61	-12.67	21.47
143 ARG CG	29.03	18.65	-13.97	21.99
143 ARG CD	28.92	19.99	-14.54	28.60
143 ARG NE	29.52	20.08	-15.87	33.70
143 ARG CZ	30.76	20.49	-16.11	33.84
143 ARG NH1	31.20	20.56	-17.36	34.28
143 ARG NH2	31.57	20.78	-15.10	32.21
143 ARG C	28.10	17.42	-10.43	24.76
143 ARG O	27.83	18.25	-9.52	25.81

Fig. 5CC

Residue Atom	X	Y	Z	B
144 THR N	27.71	16.16	-10.40	22.71
144 THR CA	26.88	15.60	-9.34	21.04
144 THR CB	26.08	14.44	-9.92	22.19
144 THR OG1	26.90	13.73	-10.86	25.50
144 THR CG2	24.89	14.96	-10.65	25.73
144 THR C	27.72	15.09	-8.16	19.87
144 THR O	27.34	14.14	-7.47	20.20
145 LEU N	28.88	15.69	-7.96	19.59
145 LEU CA	29.74	15.22	-6.88	17.69
145 LEU CB	31.22	15.48	-7.22	15.20
145 LEU CG	32.22	15.05	-6.15	16.04
145 LEU CD1	32.20	13.56	-5.96	14.53
145 LEU CD2	33.59	15.53	-6.50	13.03
145 LEU C	29.34	15.89	-5.59	17.52
145 LEU O	29.11	15.23	-4.61	20.75
146 PHE N	29.18	17.20	-5.63	17.08
146 PHE CA	28.80	17.99	-4.46	16.09
146 PHE CB	29.26	19.43	-4.70	15.22
146 PHE CG	30.77	19.58	-4.82	13.02
146 PHE CD1	31.33	20.81	-5.10	8.98
146 PHE CD2	31.62	18.49	-4.60	12.64
146 PHE CE1	32.72	20.96	-5.14	8.43
146 PHE CE2	32.99	18.63	-4.65	10.95
146 PHE CZ	33.55	19.87	-4.92	8.47
146 PHE C	27.28	17.94	-4.12	15.64
146 PHE O	26.45	18.43	-4.89	17.26
147 ALA N	26.93	17.30	-3.00	13.26
147 ALA CA	25.55	17.20	-2.55	8.71
147 ALA CB	25.41	16.04	-1.61	7.80
147 ALA C	25.10	18.50	-1.89	8.81

Fig. 5DD

Residue Atom	X	Y	Z	B
147 ALA O	24.22	19.17	-2.37	10.64
148 HIS N	25.72	18.90	-0.80	8.71
148 HIS CA	25.34	20.14	-0.15	8.60
148 HIS C	26.51	20.61	0.73	8.75
148 HIS O	27.57	20.01	0.73	9.64
148 HIS CB	24.11	19.91	0.72	7.49
148 HIS CG	24.35	18.95	1.85	10.55
148 HIS ND1	24.75	19.32	3.11	14.28
148 HIS CD2	24.25	17.60	1.89	13.72
148 HIS NE2	24.59	17.13	3.17	10.96
148 HIS CE1	24.88	18.20	3.87	11.30
149 VAL N	26.28	21.66	1.52	5.64
149 VAL CA	27.28	22.20	2.42	4.43
149 VAL CB	27.91	23.52	1.85	2.00
149 VAL CG1	27.13	24.01	0.72	2.60
149 VAL CG2	28.02	24.63	2.90	2.00
149 VAL C	26.66	22.41	3.81	5.08
149 VAL O	25.76	23.23	3.99	6.81
150 ALA N	27.07	21.63	4.79	4.31
150 ALA CA	26.54	21.77	6.12	4.19
150 ALA CB	26.61	20.47	6.82	2.00
150 ALA C	27.27	22.85	6.92	6.21
150 ALA O	28.45	23.04	6.74	8.36
151 LEU N	26.52	23.64	7.70	8.89
151 LEU CA	27.04	24.68	8.59	8.16
151 LEU CB	25.96	25.72	8.87	6.76
151 LEU CG	26.17	27.20	8.57	13.35
151 LEU CD1	26.80	27.33	7.16	14.96
151 LEU CD2	24.86	28.01	8.69	2.52
151 LEU C	27.28	23.87	9.88	10.36

Fig. 5EE

Residue Atom	X	Y	Z	B
151 LEU O	26.40	23.13	10.32	11.10
152 CYS N	28.45	23.97	10.47	10.07
152 CYS CA	28.70	23.20	11.68	10.06
152 CYS CB	29.09	21.78	11.30	9.56
152 CYS SG	30.55	21.68	10.32	12.05
152 CYS C	29.70	23.84	12.62	10.73
152 CYS O	30.22	24.91	12.35	10.79
153 ALA N	29.91	23.18	13.75	12.36
153 ALA CA	30.82	23.66	14.81	13.12
153 ALA CB	30.51	22.92	16.14	11.10
153 ALA C	32.29	23.51	14.48	12.28
153 ALA O	33.04	24.47	14.54	11.41
154 ILE N	32.67	22.27	14.19	13.17
154 ILE CA	34.04	21.91	13.84	14.44
154 ILE CB	34.76	21.20	15.06	16.21
154 ILE CG2	35.94	20.37	14.62	16.07
154 ILE CG1	35.25	22.26	16.04	18.38
154 ILE CD1	36.24	23.28	15.42	19.24
154 ILE C	33.90	20.99	12.62	14.39
154 ILE O	33.23	19.97	12.69	13.58
155 GLY N	34.40	21.47	11.48	16.35
155 GLY CA	34.31	20.72	10.24	18.21
155 GLY C	35.41	19.67	10.20	20.38
155 GLY O	36.41	19.78	10.93	21.76
156 ARG N	35.26	18.69	9.32	20.77
156 ARG CA	36.24	17.61	9.21	21.11
156 ARG CB	35.53	16.30	8.87	24.90
156 ARG CG	35.76	15.25	9.94	29.04
156 ARG CD	34.71	14.16	9.85	32.89
156 ARG NE	34.84	13.39	8.62	39.65

Fig. 5FF

Residue Atom	X	Y	Z	B
156 ARG CZ	34.67	12.06	8.54	43.91
156 ARG NH1	34.81	11.44	7.34	44.98
156 ARG NH2	34.32	11.35	9.63	42.89
156 ARG C	37.40	17.83	8.24	20.04
156 ARG O	38.31	17.01	8.18	22.30
157 ARG N	37.35	18.89	7.45	17.53
157 ARG CA	38.43	19.17	6.53	15.10
157 ARG CB	37.95	19.20	5.08	11.19
157 ARG CG	37.67	17.82	4.59	7.60
157 ARG CD	37.61	17.73	3.11	10.17
157 ARG NE	36.33	18.14	2.57	15.38
157 ARG CZ	35.39	17.30	2.14	17.80
157 ARG NH1	35.56	15.99	2.20	14.74
157 ARG NH2	34.30	17.77	1.53	18.94
157 ARG C	39.11	20.45	7.00	15.95
157 ARG O	38.48	21.29	7.67	15.82
158 LEU N	40.43	20.54	6.74	13.11
158 LEU CA	41.25	21.66	7.17	10.75
158 LEU CB	42.75	21.33	7.01	10.39
158 LEU CG	43.57	20.34	7.89	8.24
158 LEU CD1	43.12	20.23	9.32	5.72
158 LEU CD2	43.54	19.00	7.28	9.04
158 LEU C	40.95	23.00	6.55	10.71
158 LEU O	40.52	23.10	5.41	12.41
159 GLY N	41.14	24.05	7.33	9.74
159 GLY CA	40.90	25.38	6.83	11.59
159 GLY C	39.47	25.78	6.54	13.36
159 GLY O	39.19	26.92	6.09	14.85
160 THR N	38.55	24.89	6.85	12.99
160 THR CA	37.14	25.15	6.59	11.29

Fig. 5GG

Residue Atom	X	Y	Z	B
160 THR CB	36.41	23.84	6.33	13.60
160 THR OG1	36.60	22.95	7.45	13.94
160 THR CG2	36.98	23.18	5.06	14.91
160 THR C	36.45	25.93	7.68	9.45
160 THR O	35.60	25.41	8.34	10.14
161 ILE N	36.92	27.14	7.94	10.38
161 ILE CA	36.32	28.03	8.91	8.13
161 ILE CB	37.33	28.54	9.92	2.00
161 ILE CG2	36.76	29.64	10.75	3.52
161 ILE CG1	37.70	27.39	10.86	3.90
161 ILE CD1	36.64	26.97	11.81	2.00
161 ILE C	35.76	29.13	8.03	10.09
161 ILE O	36.38	29.46	6.99	10.40
162 VAL N	34.58	29.63	8.36	8.80
162 VAL CA	33.97	30.62	7.50	9.20
162 VAL CB	32.73	30.05	6.87	9.13
162 VAL CG1	33.10	28.81	6.09	4.95
162 VAL CG2	31.72	29.73	7.93	11.25
162 VAL C	33.68	31.99	8.06	11.53
162 VAL O	33.77	32.20	9.26	15.32
163 THR N	33.41	32.94	7.16	12.01
163 THR CA	33.10	34.32	7.52	10.38
163 THR CB	34.05	35.26	6.81	6.93
163 THR OG1	35.37	34.99	7.25	6.33
163 THR CG2	33.77	36.65	7.16	8.99
163 THR C	31.61	34.61	7.20	12.20
163 THR O	31.08	34.09	6.22	14.86
164 TYR N	30.91	35.31	8.10	10.65
164 TYR CA	29.49	35.65	7.94	6.92
164 TYR CB	28.59	35.17	9.10	5.68

Fig. 5HH

Residue Atom	X	Y	Z	B
164 TYR CG	28.47	33.67	9.33	5.70
164 TYR CD1	29.46	32.96	10.03	9.47
164 TYR CE1	29.36	31.57	10.24	9.65
164 TYR CD2	27.38	32.97	8.85	4.93
164 TYR CE2	27.25	31.59	9.04	4.75
164 TYR CZ	28.25	30.90	9.73	8.93
164 TYR OH	28.16	29.53	9.91	5.04
164 TYR C	29.45	37.14	7.99	6.97
164 TYR O	30.10	37.74	8.82	6.41
165 ASP N	28.63	37.72	7.13	9.42
165 ASP CA	28.46	39.14	7.07	7.63
165 ASP CB	29.69	39.78	6.52	8.26
165 ASP CG	30.01	41.06	7.23	13.00
165 ASP OD1	29.23	42.02	7.14	11.86
165 ASP OD2	31.08	41.10	7.88	18.63
165 ASP C	27.28	39.56	6.23	7.52
165 ASP O	26.80	38.82	5.39	6.42
166 THR N	26.83	40.78	6.46	7.08
166 THR CA	25.71	41.33	5.75	8.22
166 THR CB	25.04	42.46	6.57	8.96
166 THR OG1	26.03	43.39	7.02	7.50
166 THR CG2	24.31	41.90	7.76	7.28
166 THR C	26.18	41.89	4.41	9.77
166 THR O	25.66	42.87	3.94	14.12
167 SER N	27.16	41.27	3.78	10.31
167 SER CA	27.66	41.77	2.51	10.89
167 SER CB	28.41	43.07	2.73	7.08
167 SER OG	29.09	43.45	1.56	10.27
167 SER C	28.59	40.74	1.95	14.09
167 SER O	29.32	40.11	2.71	15.00

Fig. 5II

Residue Atom	X	Y	Z	B
168 LEU N	28.60	40.58	0.62	16.24
168 LEU CA	29.49	39.60	-0.02	15.71
168 LEU CB	29.15	39.44	-1.50	13.79
168 LEU CG	29.69	38.25	-2.27	9.75
168 LEU CD1	29.01	38.19	-3.57	11.59
168 LEU CD2	31.14	38.40	-2.50	14.35
168 LEU C	30.93	40.03	0.13	15.86
168 LEU O	31.75	39.26	0.57	16.44
169 ASP N	31.20	41.29	-0.19	17.47
169 ASP CA	32.53	41.86	-0.09	18.64
169 ASP CB	32.52	43.26	-0.65	19.99
169 ASP CG	31.78	43.34	-1.94	22.71
169 ASP OD1	30.59	43.72	-1.88	31.45
169 ASP OD2	32.32	42.94	-2.99	19.11
169 ASP C	33.08	41.85	1.31	18.68
169 ASP O	34.27	41.66	1.50	22.89
170 ALA N	32.23	42.09	2.30	16.76
170 ALA CA	32.65	42.06	3.68	13.79
170 ALA CB	31.62	42.68	4.52	13.68
170 ALA C	32.88	40.61	4.10	11.53
170 ALA O	33.81	40.32	4.81	12.15
171 ALA N	32.04	39.70	3.62	9.82
171 ALA CA	32.15	38.28	3.95	9.28
171 ALA CB	30.97	37.52	3.38	2.67
171 ALA C	33.44	37.70	3.42	12.12
171 ALA O	34.04	36.84	4.06	12.36
172 ILE N	33.89	38.16	2.25	13.16
172 ILE CA	35.12	37.64	1.68	13.45
172 ILE CB	35.01	37.34	0.16	14.59
172 ILE CG2	33.88	36.35	-0.11	15.84

Fig. 5JJ

Residue Atom	X	Y	Z	B
172 ILE CG1	34.84	38.60	-0.67	12.70
172 ILE CD1	35.00	38.32	-2.17	8.60
172 ILE C	36.39	38.44	1.95	13.84
172 ILE O	37.49	37.93	1.76	11.09
173 ALA N	36.25	39.68	2.43	13.69
173 ALA CA	37.41	40.53	2.74	13.94
173 ALA CB	36.97	41.93	3.20	10.45
173 ALA C	38.46	39.94	3.73	13.56
173 ALA O	39.66	40.12	3.55	13.78
174 PRO N	38.03	39.25	4.79	11.86
174 PRO CD	36.74	39.08	5.47	12.92
174 PRO CA	39.08	38.75	5.64	11.43
174 PRO CB	38.34	38.39	6.92	11.43
174 PRO CG	37.09	38.01	6.46	12.49
174 PRO C	39.80	37.59	5.03	12.85
174 PRO O	40.57	36.92	5.72	15.52
175 PHE N	39.58	37.32	3.76	13.77
175 PHE CA	40.36	36.25	3.11	15.02
175 PHE CB	39.48	35.31	2.28	15.53
175 PHE CG	38.50	34.52	3.10	10.81
175 PHE CD1	38.83	33.25	3.56	5.68
175 PHE CD2	37.26	35.09	3.44	10.26
175 PHE CE1	37.97	32.56	4.33	7.24
175 PHE CE2	36.37	34.41	4.22	5.77
175 PHE CZ	36.71	33.14	4.67	9.10
175 PHE C	41.48	36.90	2.27	13.48
175 PHE O	41.25	37.38	1.17	13.84
176 ARG N	42.67	36.92	2.81	13.55
176 ARG CA	43.80	37.56	2.17	17.04
176 ARG CB	44.73	38.05	3.26	19.56

Fig. 5KK

Residue Atom	X	Y	Z	B
176 ARG CG	44.00	38.69	4.44	20.17
176 ARG CD	43.62	40.15	4.20	17.77
176 ARG NE	42.54	40.54	5.10	16.71
176 ARG CZ	42.40	41.73	5.65	16.08
176 ARG NH1	41.38	41.98	6.45	18.13
176 ARG NH2	43.26	42.68	5.42	18.59
176 ARG C	44.57	36.76	1.08	18.45
176 ARG O	45.12	37.33	0.12	17.41
177 HIS N	44.64	35.43	1.24	19.20
177 HIS CA	45.31	34.60	0.25	19.47
177 HIS CB	45.95	33.38	0.90	23.19
177 HIS CG	46.60	33.67	2.21	25.40
177 HIS CD2	46.85	32.87	3.27	28.95
177 HIS ND1	47.06	34.92	2.55	26.63
177 HIS CE1	47.55	34.89	3.78	29.03
177 HIS NE2	47.44	33.66	4.24	31.80
177 HIS C	44.21	34.13	-0.66	18.10
177 HIS O	43.68	33.06	-0.46	19.23
178 LEU N	43.80	34.95	-1.61	17.55
178 LEU CA	42.74	34.54	-2.51	16.48
178 LEU CB	41.42	35.15	-2.05	13.16
178 LEU CG	40.15	34.33	-2.15	11.21
178 LEU CD1	40.42	33.03	-1.48	12.21
178 LEU CD2	39.03	35.04	-1.46	11.79
178 LEU C	43.14	35.11	-3.85	19.60
178 LEU O	43.65	36.24	-3.94	23.82
179 ASP N	43.00	34.32	-4.91	18.49
179 ASP CA	43.35	34.83	-6.21	18.94
179 ASP CB	43.21	33.72	-7.24	17.14
179 ASP CG	43.87	34.04	-8.54	19.35

Fig. 5LL

Residue Atom	X	Y	Z	B
179 ASP OD1	43.91	35.21	-8.99	19.23
179 ASP OD2	44.34	33.08	-9.16	25.64
179 ASP C	42.41	35.99	-6.56	20.51
179 ASP O	41.25	36.01	-6.14	20.70
180 PRO N	42.93	37.03	-7.23	22.33
180 PRO CD	44.34	37.44	-7.40	21.14
180 PRO CA	42.01	38.13	-7.58	22.11
180 PRO CB	42.91	39.08	-8.35	21.42
180 PRO CG	44.22	38.93	-7.60	23.42
180 PRO C	40.90	37.59	-8.47	21.04
180 PRO O	39.75	38.01	-8.38	22.35
181 ALA N	41.26	36.64	-9.33	19.96
181 ALA CA	40.34	36.01	-10.26	16.55
181 ALA CB	41.06	35.00	-11.14	16.69
181 ALA C	39.25	35.33	-9.46	17.10
181 ALA O	38.12	35.24	-9.93	18.74
182 THR N	39.58	34.87	-8.26	15.61
182 THR CA	38.58	34.21	-7.43	14.74
182 THR CB	39.22	33.42	-6.29	13.42
182 THR OG1	40.19	32.53	-6.83	12.41
182 THR CG2	38.18	32.62	-5.56	11.92
182 THR C	37.63	35.25	-6.88	14.68
182 THR O	36.44	35.07	-6.93	14.89
183 ARG N	38.17	36.36	-6.41	13.14
183 ARG CA	37.34	37.44	-5.91	14.88
183 ARG CB	38.22	38.62	-5.50	14.78
183 ARG CG	38.77	38.50	-4.13	14.46
183 ARG CD	40.14	38.98	-4.07	20.35
183 ARG NE	40.91	38.18	-3.12	29.90
183 ARG CZ	41.59	38.66	-2.07	32.97

Fig. 5MM

Residue Atom	X	Y	Z	B
183 ARG NH1	42.28	37.84	-1.27	30.33
183 ARG NH2	41.63	39.96	-1.82	33.84
183 ARG C	36.32	37.88	-6.97	17.05
183 ARG O	35.10	37.76	-6.82	18.36
184 GLU N	36.82	38.36	-8.09	19.71
184 GLU CA	35.94	38.82	-9.14	23.15
184 GLU CB	36.76	39.63	-10.16	26.44
184 GLU CG	37.22	41.00	-9.56	30.83
184 GLU CD	36.11	42.11	-9.63	30.38
184 GLU OE1	35.60	42.59	-8.60	26.77
184 GLU OE2	35.76	42.49	-10.77	35.03
184 GLU C	35.03	37.75	-9.78	21.57
184 GLU O	33.93	38.05	-10.25	20.27
185 GLY N	35.48	36.50	-9.75	20.10
185 GLY CA	34.69	35.43	-10.34	19.41
185 GLY C	33.49	35.10	-9.48	18.47
185 GLY O	32.36	35.08	-9.95	18.35
186 VAL N	33.75	34.88	-8.21	19.84
186 VAL CA	32.72	34.55	-7.24	19.69
186 VAL CB	33.37	34.12	-5.91	21.04
186 VAL CG1	33.57	35.33	-5.00	20.42
186 VAL CG2	32.57	32.99	-5.25	20.27
186 VAL C	31.78	35.73	-7.03	19.38
186 VAL O	30.69	35.57	-6.49	20.08
187 ARG N	32.22	36.91	-7.41	19.63
187 ARG CA	31.38	38.10	-7.29	19.57
187 ARG CB	32.20	39.38	-7.27	17.68
187 ARG CG	32.83	39.74	-5.95	16.17
187 ARG CD	32.88	41.25	-5.92	17.78
187 ARG NE	33.99	41.87	-5.20	16.37

Fig. 5NN

Residue Atom	X	Y	Z	B
187 ARG CZ	35.27	41.69	-5.49	15.62
187 ARG NH1	36.21	42.30	-4.80	12.01
187 ARG NH2	35.60	40.84	-6.44	16.94
187 ARG C	30.32	38.18	-8.41	20.06
187 ARG O	29.24	38.71	-8.20	22.75
188 ARG N	30.64	37.72	-9.61	19.80
188 ARG CA	29.64	37.74	-10.66	21.24
188 ARG CB	30.22	37.59	-12.04	22.69
188 ARG CG	31.14	38.67	-12.45	28.10
188 ARG CD	31.87	38.20	-13.69	31.07
188 ARG NE	32.28	36.81	-13.53	32.08
188 ARG CZ	31.71	35.78	-14.17	32.73
188 ARG NH1	32.14	34.53	-13.96	29.41
188 ARG NH2	30.70	36.03	-15.03	34.51
188 ARG C	28.67	36.60	-10.45	21.19
188 ARG O	27.47	36.86	-10.39	24.79
189 GLU N	29.14	35.36	-10.35	18.68
189 GLU CA	28.21	34.26	-10.15	19.63
189 GLU CB	28.89	32.91	-9.92	22.18
189 GLU CG	29.77	32.37	-11.04	27.60
189 GLU CD	31.02	31.65	-10.49	30.89
189 GLU OE1	32.13	32.22	-10.60	33.41
189 GLU OE2	30.90	30.54	-9.91	30.22
189 GLU C	27.27	34.52	-8.98	18.60
189 GLU O	26.08	34.29	-9.09	21.78
190 ALA N	27.79	35.06	-7.89	17.44
190 ALA CA	26.96	35.35	-6.71	16.93
190 ALA CB	27.81	35.93	-5.62	15.50
190 ALA C	25.74	36.24	-6.95	17.54
190 ALA O	24.67	35.98	-6.41	16.72

Fig. 500

Residue Atom	X	Y	Z	B
191 ALA N	25.91	37.29	-7.77	19.33
191 ALA CA	24.84	38.26	-8.12	19.45
191 ALA CB	25.43	39.45	-8.78	18.90
191 ALA C	23.79	37.65	-9.03	19.65
191 ALA O	22.58	37.75	-8.81	20.16
192 GLU N	24.27	37.01	-10.07	20.37
192 GLU CA	23.40	36.35	-11.01	22.48
192 GLU CB	24.21	35.64	-12.05	25.16
192 GLU CG	25.14	36.54	-12.76	33.62
192 GLU CD	25.82	35.84	-13.91	41.14
192 GLU OE1	26.84	36.41	-14.39	47.35
192 GLU OE2	25.34	34.73	-14.35	41.85
192 GLU C	22.54	35.34	-10.30	22.43
192 GLU O	21.36	35.21	-10.61	23.12
193 ALA N	23.13	34.61	-9.36	21.17
193 ALA CA	22.40	33.60	-8.63	21.73
193 ALA CB	23.30	32.71	-7.90	21.96
193 ALA C	21.42	34.24	-7.68	23.53
193 ALA O	20.34	33.69	-7.46	26.65
194 GLU N	21.74	35.40	-7.13	23.26
194 GLU CA	20.80	36.02	-6.21	22.79
194 GLU CB	21.38	37.27	-5.59	22.73
194 GLU CG	22.50	36.97	-4.72	24.60
194 GLU CD	22.71	38.07	-3.75	29.85
194 GLU OE1	23.31	39.09	-4.14	32.69
194 GLU OE2	22.27	37.91	-2.58	34.29
194 GLU C	19.54	36.37	-6.96	23.63
194 GLU O	18.43	36.33	-6.41	25.04
195 LEU N	19.71	36.71	-8.24	24.06
195 LEU CA	18.60	37.05	-9.10	23.45

Fig. 5PP

Residue Atom	X	Y	Z	B
195 LEU CB	19.10	37.53	-10.45	24.46
195 LEU CG	19.80	38.89	-10.41	24.17
195 LEU CD1	20.24	39.34	-11.80	25.83
195 LEU CD2	18.86	39.91	-9.83	24.72
195 LEU C	17.61	35.88	-9.24	23.50
195 LEU O	16.48	36.08	-9.62	25.60
196 ALA N	18.05	34.66	-8.98	23.27
196 ALA CA	17.11	33.55	-9.05	23.63
196 ALA CB	17.82	32.23	-9.30	24.34
196 ALA C	16.39	33.52	-7.72	24.88
196 ALA O	15.17	33.51	-7.70	29.50
197 LEU N	17.13	33.55	-6.61	23.36
197 LEU CA	16.52	33.54	-5.29	22.81
197 LEU CB	17.55	33.72	-4.17	20.76
197 LEU CG	18.29	32.43	-3.83	16.68
197 LEU CD1	17.28	31.35	-3.70	17.98
197 LEU CD2	19.23	32.06	-4.95	16.49
197 LEU C	15.41	34.59	-5.20	24.66
197 LEU O	14.42	34.41	-4.48	26.15
198 ALA N	15.60	35.71	-5.88	23.99
198 ALA CA	14.57	36.73	-5.91	24.22
198 ALA CB	13.48	36.28	-6.85	24.94
198 ALA C	13.94	37.20	-4.60	24.56
198 ALA O	13.04	38.04	-4.61	26.75
199 GLY N	14.45	36.75	-3.46	24.14
199 GLY CA	13.86	37.18	-2.20	22.52
199 GLY C	13.29	35.97	-1.50	21.30
199 GLY O	12.35	36.06	-0.69	21.69
200 ARG N	13.82	34.81	-1.87	18.31
200 ARG CA	13.40	33.56	-1.29	15.04

Fig. 5QQ

Residue Atom	X	Y	Z	B
200 ARG CB	14.13	32.45	-2.00	12.08
200 ARG CG	13.33	31.23	-2.17	16.15
200 ARG CD	13.80	30.12	-1.30	17.37
200 ARG NE	14.08	28.96	-2.13	16.81
200 ARG CZ	14.00	27.71	-1.72	17.20
200 ARG NH1	14.27	26.73	-2.55	19.87
200 ARG NH2	13.66	27.46	-0.46	19.95
200 ARG C	13.85	33.59	0.15	14.28
200 ARG O	14.75	34.33	0.50	15.36
201 THR N	13.25	32.78	0.99	13.05
201 THR CA	13.66	32.76	2.37	11.06
201 THR CB	12.87	33.75	3.14	12.97
201 THR OG1	13.24	35.05	2.66	17.96
201 THR CG2	13.14	33.64	4.67	14.46
201 THR C	13.41	31.38	2.86	9.58
201 THR O	12.58	30.66	2.31	13.25
202 TRP N	14.21	30.95	3.82	3.78
202 TRP CA	14.04	29.65	4.35	3.74
202 TRP CB	15.39	28.98	4.43	2.42
202 TRP CG	15.90	28.63	3.02	3.24
202 TRP CD2	16.45	29.52	2.06	2.00
202 TRP CE2	16.70	28.78	0.90	2.00
202 TRP CE3	16.75	30.88	2.07	6.37
202 TRP CD1	15.85	27.40	2.42	2.00
202 TRP NE1	16.33	27.49	1.14	2.00
202 TRP CZ2	17.23	29.35	-0.24	2.00
202 TRP CZ3	17.29	31.45	0.93	4.03
202 TRP CH2	17.52	30.69	-0.21	5.11
202 TRP C	13.29	29.73	5.65	5.38
202 TRP O	13.29	30.78	6.27	7.63

Fig. 5RR

Residue Atom	X	Y	Z	B
203 ALA N	12.51	28.70	5.95	5.73
203 ALA CA	11.71	28.64	7.18	6.91
203 ALA CB	10.37	29.27	6.96	2.00
203 ALA C	11.55	27.18	7.62	9.43
203 ALA O	10.45	26.63	7.70	11.74
204 PRO N	12.66	26.53	7.97	9.34
204 PRO CD	14.00	27.11	8.21	6.42
204 PRO CA	12.63	25.14	8.39	7.43
204 PRO CB	14.10	24.87	8.72	4.23
204 PRO CG	14.59	26.18	9.20	3.30
204 PRO C	11.71	24.83	9.57	8.06
204 PRO O	11.29	23.70	9.71	9.66
205 GLY N	11.45	25.81	10.45	9.18
205 GLY CA	10.61	25.63	11.63	9.18
205 GLY C	11.41	25.82	12.90	8.97
205 GLY O	12.38	25.10	13.10	9.01
206 VAL N	10.99	26.71	13.80	7.76
206 VAL CA	11.82	26.92	14.97	9.21
206 VAL CB	11.49	28.20	15.86	7.78
206 VAL CG1	10.94	29.36	15.05	4.18
206 VAL CG2	10.66	27.87	17.04	5.53
206 VAL C	12.14	25.71	15.81	11.82
206 VAL O	13.27	25.56	16.20	14.86
207 GLU N	11.23	24.79	16.05	13.45
207 GLU CA	11.65	23.65	16.87	16.00
207 GLU CB	10.46	22.93	17.53	20.19
207 GLU CG	9.67	23.76	18.59	26.38
207 GLU CD	10.54	24.73	19.45	30.51
207 GLU OE1	11.35	24.27	20.29	29.04
207 GLU OE2	10.39	25.97	19.31	32.60

Fig. 5SS

Residue Atom	X	Y	Z	B
207 GLU C	12.60	22.65	16.18	15.39
207 GLU O	13.30	21.91	16.87	15.80
208 ALA N	12.61	22.61	14.85	13.40
208 ALA CA	13.51	21.73	14.09	10.45
208 ALA CB	13.13	21.64	12.63	9.96
208 ALA C	14.87	22.38	14.23	10.25
208 ALA O	15.86	21.68	14.40	12.17
209 LEU N	14.90	23.72	14.16	8.37
209 LEU CA	16.14	24.50	14.32	7.08
209 LEU CB	15.92	25.99	14.07	2.00
209 LEU CG	15.89	26.40	12.61	2.00
209 LEU CD1	15.68	27.88	12.43	2.00
209 LEU CD2	17.20	26.00	12.02	6.01
209 LEU C	16.66	24.32	15.75	8.22
209 LEU O	17.79	23.95	15.96	9.00
210 THR N	15.79	24.58	16.72	9.20
210 THR CA	16.11	24.43	18.13	10.30
210 THR CB	14.85	24.69	18.97	11.52
210 THR OG1	14.38	26.02	18.71	14.04
210 THR CG2	15.15	24.57	20.43	12.38
210 THR C	16.65	23.02	18.42	11.22
210 THR O	17.66	22.86	19.07	11.57
211 HIS N	15.98	22.00	17.92	13.49
211 HIS CA	16.43	20.65	18.14	15.52
211 HIS CB	15.38	19.62	17.68	20.64
211 HIS CG	14.24	19.40	18.64	26.90
211 HIS CD2	12.90	19.58	18.49	27.65
211 HIS ND1	14.41	18.93	19.93	29.22
211 HIS CE1	13.24	18.84	20.53	28.12
211 HIS NE2	12.30	19.22	19.68	28.69

Fig. 5TT

Residue Atom	X	Y	Z	B
211 HIS C	17.77	20.39	17.47	16.33
211 HIS O	18.56	19.58	17.95	20.48
212 THR N	18.05	21.06	16.35	13.98
212 THR CA	19.32	20.84	15.65	11.93
212 THR CB	19.15	21.12	14.16	9.12
212 THR OG1	18.02	20.38	13.70	8.08
212 THR CG2	20.36	20.66	13.39	9.84
212 THR C	20.54	21.58	16.26	12.09
212 THR O	21.67	21.06	16.32	12.03
213 LEU N	20.31	22.80	16.74	10.65
213 LEU CA	21.32	23.57	17.38	9.64
213 LEU CB	20.81	24.98	17.55	6.93
213 LEU CG	20.72	25.73	16.22	6.38
213 LEU CD1	20.09	27.11	16.40	5.81
213 LEU CD2	22.10	25.88	15.62	4.84
213 LEU C	21.70	22.91	18.74	12.82
213 LEU O	22.88	22.87	19.11	12.94
214 LEU N	20.73	22.34	19.45	12.13
214 LEU CA	21.04	21.67	20.71	10.23
214 LEU CB	19.77	21.15	21.41	9.12
214 LEU CG	19.70	20.84	22.94	9.66
214 LEU CD1	19.43	19.41	23.18	8.62
214 LEU CD2	20.96	21.26	23.71	10.58
214 LEU C	21.97	20.51	20.37	11.45
214 LEU O	23.05	20.39	20.94	9.53
215 SER N	21.58	19.71	19.38	13.87
215 SER CA	22.34	18.52	18.93	12.55
215 SER CB	21.62	17.82	17.80	12.82
215 SER OG	22.33	16.68	17.38	11.94
215 SER C	23.79	18.82	18.54	10.44

Fig. 5UU

Residue Atom	X	Y	Z	B
215 SER O	24.65	17.93	18.59	7.88
216 THR N	24.04	20.04	18.10	9.57
216 THR CA	25.40	20.46	17.78	11.80
216 THR CB	25.38	21.81	17.13	10.37
216 THR OG1	24.95	21.63	15.79	16.81
216 THR CG2	26.72	22.46	17.14	8.20
216 THR C	26.17	20.53	19.11	13.58
216 THR O	27.18	19.86	19.29	15.60
217 ALA N	25.61	21.25	20.07	13.36
217 ALA CA	26.22	21.39	21.37	10.87
217 ALA CB	25.39	22.25	22.23	11.37
217 ALA C	26.39	20.05	22.04	10.76
217 ALA O	27.41	19.80	22.65	12.12
218 VAL N	25.39	19.19	21.94	11.01
218 VAL CA	25.50	17.91	22.61	10.40
218 VAL CB	24.15	17.17	22.73	7.87
218 VAL CG1	24.38	15.75	23.14	2.00
218 VAL CG2	23.30	17.83	23.77	9.41
218 VAL C	26.51	17.04	21.95	12.12
218 VAL O	27.44	16.59	22.59	13.85
219 ASN N	26.38	16.86	20.65	14.27
219 ASN CA	27.31	15.99	19.95	15.70
219 ASN CB	26.84	15.77	18.53	16.16
219 ASN CG	25.63	14.91	18.45	17.91
219 ASN OD1	25.65	13.75	18.89	18.27
219 ASN ND2	24.57	15.45	17.89	18.83
219 ASN C	28.76	16.45	19.98	15.95
219 ASN O	29.67	15.67	19.77	16.48
220 ASN N	28.97	17.70	20.36	16.79
220 ASN CA	30.31	18.24	20.38	18.70

Fig. 5VV

Residue Atom	X	Y	Z	B
220 ASN CB	30.38	19.53	19.54	21.43
220 ASN CG	30.40	19.26	18.06	23.36
220 ASN OD1	31.38	18.73	17.56	25.24
220 ASN ND2	29.32	19.61	17.36	22.89
220 ASN C	30.82	18.58	21.75	19.42
220 ASN O	31.87	19.23	21.85	20.88
221 MET N	30.09	18.16	22.80	19.08
221 MET CA	30.46	18.48	24.19	16.02
221 MET CB	29.34	18.12	25.18	11.71
221 MET CG	29.13	16.64	25.30	7.04
221 MET SD	27.78	16.27	26.31	12.68
221 MET CE	27.78	14.54	26.24	5.67
221 MET C	31.77	17.87	24.65	15.97
221 MET O	32.38	18.40	25.56	17.74
222 MET N	32.19	16.79	24.00	15.13
222 MET CA	33.43	16.08	24.33	15.50
222 MET CB	33.30	14.65	23.86	14.49
222 MET CG	32.34	13.93	24.74	13.32
222 MET SD	32.51	14.48	26.50	14.19
222 MET CE	32.06	12.88	27.24	8.26
222 MET C	34.78	16.69	23.90	17.78
222 MET O	35.85	16.39	24.46	17.28
223 LEU N	34.75	17.54	22.89	19.11
223 LEU CA	35.94	18.21	22.43	16.60
223 LEU CB	35.61	19.13	21.25	16.31
223 LEU CG	35.57	18.53	19.84	15.40
223 LEU CD1	34.35	17.66	19.66	17.38
223 LEU CD2	35.58	19.61	18.79	14.99
223 LEU C	36.60	19.01	23.56	18.12
223 LEU O	36.03	19.93	24.16	17.20

Fig. 5WW

Residue Atom	X	Y	Z	B
224 ARG N	37.78	18.54	23.91	22.06
224 ARG CA	38.64	19.19	24.90	24.12
224 ARG CB	39.73	18.20	25.29	23.20
224 ARG CG	39.12	16.87	25.81	28.37
224 ARG CD	38.67	16.97	27.29	29.88
224 ARG NE	37.37	16.38	27.72	31.45
224 ARG CZ	36.71	15.32	27.20	31.68
224 ARG NH1	35.56	14.94	27.75	28.69
224 ARG NH2	37.14	14.67	26.12	32.52
224 ARG C	39.12	20.36	24.02	25.20
224 ARG O	39.76	20.18	22.98	25.52
225 ASP N	38.62	21.54	24.36	26.60
225 ASP CA	38.82	22.77	23.58	27.04
225 ASP CB	39.87	23.73	24.12	29.55
225 ASP CG	39.45	25.20	23.94	32.91
225 ASP OD1	38.28	25.44	23.55	32.59
225 ASP OD2	40.27	26.11	24.21	36.97
225 ASP C	38.83	22.71	22.05	26.34
225 ASP O	39.69	22.11	21.40	24.27
226 ARG N	37.80	23.32	21.50	25.04
226 ARG CA	37.64	23.36	20.07	25.34
226 ARG CB	36.18	23.15	19.68	28.06
226 ARG CG	35.21	24.15	20.36	30.00
226 ARG CD	33.98	24.48	19.49	28.19
226 ARG NE	33.30	25.67	19.99	27.27
226 ARG CZ	32.73	26.59	19.23	25.17
226 ARG NH1	32.16	27.64	19.79	25.45
226 ARG NH2	32.73	26.46	17.91	26.06
226 ARG C	38.12	24.72	19.64	23.86
226 ARG O	38.23	24.98	18.43	23.14

Fig. 5XX

Residue Atom	X	Y	Z	B
227 TRP N	38.36	25.59	20.61	20.47
227 TRP CA	38.86	26.92	20.29	20.99
227 TRP CB	38.83	27.82	21.52	24.01
227 TRP CG	37.47	28.34	21.84	29.39
227 TRP CD2	36.61	29.13	20.99	29.25
227 TRP CE2	35.45	29.44	21.73	29.90
227 TRP CE3	36.72	29.61	19.67	29.32
227 TRP CD1	36.81	28.21	23.03	31.69
227 TRP NE1	35.60	28.87	22.97	32.92
227 TRP CZ2	34.41	30.21	21.21	29.51
227 TRP CZ3	35.68	30.37	19.15	28.34
227 TRP CH2	34.54	30.66	19.92	30.27
227 TRP C	40.28	26.88	19.70	21.14
227 TRP O	40.70	27.78	18.98	23.66
228 SER N	41.02	25.82	20.02	18.16
228 SER CA	42.35	25.67	19.51	15.93
228 SER CB	43.01	24.60	20.32	16.29
228 SER OG	42.49	24.70	21.62	19.84
228 SER C	42.25	25.29	18.02	17.85
228 SER O	42.97	25.85	17.17	20.25
229 LEU N	41.33	24.36	17.71	14.42
229 LEU CA	41.09	23.92	16.36	10.55
229 LEU CB	40.08	22.81	16.38	9.10
229 LEU CG	40.63	21.50	16.89	11.53
229 LEU CD1	39.52	20.48	17.04	10.67
229 LEU CD2	41.66	21.00	15.92	13.85
229 LEU C	40.52	25.09	15.57	11.38
229 LEU O	40.93	25.36	14.46	13.27
230 VAL N	39.59	25.80	16.15	11.63
230 VAL CA	39.03	26.94	15.44	10.61

Fig. 5YY

Residue Atom	X	Y	Z	B
230 VAL CB	37.97	27.70	16.30	7.94
230 VAL CG1	37.50	28.94	15.62	2.00
230 VAL CG2	36.80	26.80	16.56	6.47
230 VAL C	40.19	27.84	15.03	11.91
230 VAL O	40.41	28.04	13.83	14.51
231 ALA N	41.02	28.24	15.99	12.11
231 ALA CA	42.16	29.11	15.71	12.32
231 ALA CB	42.83	29.52	16.97	7.72
231 ALA C	43.19	28.58	14.70	13.21
231 ALA O	43.59	29.29	13.79	14.39
232 GLU N	43.59	27.33	14.85	13.83
232 GLU CA	44.56	26.72	13.95	12.96
232 GLU CB	44.93	25.34	14.50	11.20
232 GLU CG	45.60	24.47	13.51	19.11
232 GLU CD	45.15	23.00	13.59	25.85
232 GLU OE1	45.99	22.16	14.01	27.20
232 GLU OE2	43.98	22.67	13.21	25.73
232 GLU C	44.01	26.67	12.50	13.22
232 GLU O	44.78	26.81	11.53	14.62
233 ARG N	42.68	26.56	12.39	11.85
233 ARG CA	41.95	26.50	11.11	9.70
233 ARG CB	40.61	25.83	11.26	6.48
233 ARG CG	40.65	24.48	11.84	10.11
233 ARG CD	41.18	23.46	10.91	13.64
233 ARG NE	40.24	22.35	10.76	15.30
233 ARG CZ	39.98	21.45	11.70	14.92
233 ARG NH1	39.12	20.46	11.47	14.87
233 ARG NH2	40.59	21.53	12.88	19.60
233 ARG C	41.71	27.89	10.56	8.03
233 ARG O	41.72	28.07	9.36	9.31

Fig. 5ZZ

Residue Atom	X	Y	Z	B
234 ARG N	41.40	28.85	11.43	5.29
234 ARG CA	41.23	30.21	10.97	8.12
234 ARG CB	40.99	31.17	12.15	9.61
234 ARG CG	41.12	32.63	11.76	13.36
234 ARG CD	40.99	33.66	12.86	19.39
234 ARG NE	41.13	35.02	12.27	31.29
234 ARG CZ	40.78	36.20	12.83	34.64
234 ARG NH1	40.22	36.27	14.06	34.94
234 ARG NH2	41.11	37.34	12.19	33.68
234 ARG C	42.56	30.53	10.26	11.77
234 ARG O	42.58	31.07	9.15	14.61
235 ARG N	43.68	30.16	10.89	13.57
235 ARG CA	45.04	30.34	10.36	13.19
235 ARG CB	46.06	29.70	11.30	15.90
235 ARG CG	46.65	30.65	12.33	21.17
235 ARG CD	47.32	29.87	13.48	28.37
235 ARG NE	48.05	28.64	13.04	34.85
235 ARG CZ	48.35	27.59	13.84	35.90
235 ARG NH1	49.03	26.54	13.34	33.53
235 ARG NH2	47.99	27.57	15.13	33.79
235 ARG C	45.16	29.70	8.99	11.79
235 ARG O	45.43	30.38	8.01	10.49
236 GLN N	44.97	28.39	8.93	10.68
236 GLN CA	45.05	27.66	7.67	11.39
236 GLN CB	44.43	26.28	7.82	12.95
236 GLN CG	45.38	25.22	8.35	15.41
236 GLN CD	44.68	24.20	9.21	19.29
236 GLN OE1	43.46	24.27	9.42	22.58
236 GLN NE2	45.44	23.23	9.72	16.75
236 GLN C	44.41	28.41	6.51	11.05

Fig. 5AAA

Residue Atom	X	Y	Z	B
236 GLN O	45.10	28.82	5.61	12.47
237 ALA N	43.10	28.63	6.58	11.48
237 ALA CA	42.32	29.35	5.57	12.32
237 ALA CB	40.88	29.54	6.09	9.54
237 ALA C	42.97	30.72	5.19	13.34
237 ALA O	42.85	31.22	4.06	13.35
238 GLY N	43.65	31.32	6.14	12.66
238 GLY CA	44.29	32.59	5.88	11.36
238 GLY C	43.37	33.74	6.12	10.86
238 GLY O	43.43	34.72	5.38	12.92
239 ILE N	42.55	33.64	7.16	10.68
239 ILE CA	41.60	34.70	7.51	11.68
239 ILE CB	40.36	34.16	8.28	10.27
239 ILE CG2	39.49	35.30	8.79	10.05
239 ILE CG1	39.53	33.25	7.38	8.25
239 ILE CD1	38.76	32.25	8.14	10.93
239 ILE C	42.33	35.70	8.38	14.80
239 ILE O	43.02	35.35	9.33	14.06
240 ALA N	42.24	36.96	8.00	17.15
240 ALA CA	42.88	38.00	8.75	20.17
240 ALA CB	43.68	38.87	7.81	22.58
240 ALA C	41.71	38.77	9.31	22.83
240 ALA O	40.68	38.19	9.62	26.27
241 GLY N	41.88	40.06	9.52	25.88
241 GLY CA	40.77	40.86	9.95	28.69
241 GLY C	40.33	40.95	11.39	29.43
241 GLY O	40.80	40.26	12.29	27.82
242 HIS N	39.40	41.89	11.56	31.35
242 HIS CA	38.73	42.29	12.79	30.69
242 HIS CB	38.60	43.82	12.72	32.80

Fig. 5BBB

Residue Atom	X	Y	Z	B
242 HIS CG	38.00	44.46	13.93	33.44
242 HIS CD2	37.82	45.77	14.24	34.70
242 HIS ND1	37.46	43.75	14.98	35.41
242 HIS CE1	36.98	44.59	15.88	35.13
242 HIS NE2	37.17	45.82	15.45	33.22
242 HIS C	37.34	41.58	12.68	30.07
242 HIS O	36.27	42.22	12.55	30.34
243 THR N	37.42	40.25	12.69	27.31
243 THR CA	36.29	39.35	12.60	26.00
243 THR CB	36.78	37.90	12.31	28.51
243 THR OG1	37.38	37.37	13.51	30.37
243 THR OG2	37.80	37.84	11.15	27.57
243 THR C	35.55	39.27	13.91	24.69
243 THR O	36.01	39.77	14.94	26.56
244 TYR N	34.38	38.63	13.86	22.67
244 TYR CA	33.53	38.43	15.03	19.67
244 TYR CB	32.07	38.16	14.60	12.48
244 TYR CG	31.38	39.31	13.93	4.66
244 TYR CD1	31.42	39.46	12.55	7.44
244 TYR CE1	30.78	40.51	11.91	4.93
244 TYR CD2	30.68	40.23	14.67	5.71
244 TYR CE2	30.04	41.29	14.07	7.76
244 TYR CZ	30.08	41.43	12.70	10.20
244 TYR OH	29.41	42.52	12.16	16.33
244 TYR C	34.05	37.21	15.81	20.03
244 TYR O	33.75	37.05	16.99	22.51
245 LEU N	34.85	36.38	15.15	18.64
245 LEU CA	35.35	35.15	15.74	17.77
245 LEU CB	35.90	34.29	14.60	13.77
245 LEU CG	36.22	32.85	14.88	12.70

Fig. 5CCC

Residue Atom	X	Y	Z	B
245 LEU CD1	34.93	32.10	14.96	9.99
245 LEU CD2	37.07	32.32	13.76	12.02
245 LEU C	36.39	35.37	16.84	18.62
245 LEU O	37.44	35.96	16.60	21.44
246 GLN N	36.11	34.90	18.05	18.72
246 GLN CA	37.04	35.09	19.17	20.51
246 GLN CB	36.28	35.10	20.51	20.38
246 GLN CG	34.94	35.80	20.50	21.11
246 GLN CD	35.00	37.32	20.62	19.51
246 GLN OE1	34.89	37.85	21.71	19.14
246 GLN NE2	35.11	38.02	19.48	13.60
246 GLN C	38.12	33.99	19.18	21.66
246 GLN O	38.33	33.30	20.20	23.64
247 ALA N	38.78	33.82	18.04	21.35
247 ALA CA	39.82	32.83	17.85	20.56
247 ALA CB	39.28	31.42	17.98	17.52
247 ALA C	40.31	33.09	16.43	23.39
247 ALA O	41.37	32.52	16.09	27.93
247 ALA OT	39.70	33.90	15.69	22.64
301 WAT OH2	18.08	35.78	8.28	4.83
302 WAT OH2	46.30	24.32	-0.62	2.00
303 WAT OH2	42.26	21.71	-12.75	9.96
304 WAT OH2	29.16	25.07	19.50	12.46
305 WAT OH2	40.30	41.06	1.38	9.27
306 WAT OH2	43.02	20.55	13.31	8.53
307 WAT OH2	31.60	24.18	39.04	11.92
308 WAT OH2	44.97	16.87	1.77	11.06
309 WAT OH2	46.56	26.96	1.84	17.18
310 WAT OH2	39.10	38.80	-0.17	14.70
311 WAT OH2	13.79	29.75	-5.95	4.60

Fig. 5DDD

Residue Atom	X	Y	Z	B
312 WAT OH2	19.29	20.32	2.86	17.45
313 WAT OH2	38.55	38.56	16.92	9.84
314 WAT OH2	40.37	25.41	46.65	9.57
315 WAT OH2	28.73	43.64	9.47	8.54
316 WAT OH2	28.63	20.63	14.19	7.23
317 WAT OH2	36.01	35.30	23.39	21.88
318 WAT OH2	29.89	36.21	28.21	20.83
319 WAT OH2	46.03	18.98	-4.95	19.25
320 WAT OH2	43.26	18.57	1.32	11.00
321 WAT OH2	34.16	20.32	7.14	15.58
322 WAT OH2	39.89	14.13	37.97	20.48
323 WAT OH2	40.43	21.05	3.53	26.12
324 WAT OH2	38.65	17.74	12.52	22.99
325 WAT OH2	13.54	17.29	5.31	22.94
326 WAT OH2	20.17	15.73	2.01	29.37
327 WAT OH2	3.49	7.49	39.34	20.46
328 WAT OH2	31.98	14.24	1.64	26.83
329 WAT OH2	5.50	12.64	32.21	27.11
330 WAT OH2	5.64	16.70	45.62	11.34
331 WAT OH2	28.48	17.59	11.13	39.80
332 WAT OH2	14.11	16.60	15.62	25.28
333 WAT OH2	8.97	13.57	32.58	29.38

Fig. 6A

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
61	HIS N	-12.45	-4.14	6.98	30.00
61	HIS CA	-13.09	-5.29	7.68	30.00
61	HIS CB	-13.58	-6.34	6.67	30.00
61	HIS CG	-14.61	-5.80	5.72	30.00
61	HIS CD2	-14.77	-4.58	5.17	30.00
61	HIS ND1	-15.59	-6.59	5.17	30.00
61	HIS CE1	-16.31	-5.88	4.32	30.00
61	HIS NE2	-15.84	-4.65	4.30	30.00
61	HIS C	-12.35	-5.97	8.84	30.00
61	HIS O	-12.85	-6.93	9.45	30.00
129	SER N	-17.57	-0.53	1.82	30.00
129	SER CA	-17.87	-1.90	1.55	30.00
129	SER CB	-16.59	-2.67	1.72	30.00
129	SER OG	-16.86	-4.06	1.63	30.00
129	SER C	-18.86	-2.27	2.69	30.00
129	SER O	-18.55	-2.30	3.78	30.00
131	ALA N	-21.18	-4.82	4.64	30.00
131	ALA CA	-21.24	-6.27	4.85	30.00
131	ALA CB	-20.27	-6.70	5.94	30.00
131	ALA C	-22.65	-6.66	5.32	30.00
131	ALA O	-23.26	-5.92	6.11	30.00
148	HIS N	-22.28	-4.06	8.86	30.00
148	HIS CA	-21.39	-2.88	9.07	30.00
148	HIS CB	-20.28	-3.23	10.04	30.00
148	HIS CG	-19.42	-4.37	9.58	30.00
148	HIS CD2	-19.55	-5.71	9.74	30.00
148	HIS ND1	-18.23	-4.18	8.90	30.00
148	HIS CE1	-17.67	-5.35	8.66	30.00
148	HIS NE2	-18.45	-6.30	9.16	30.00
148	HIS C	-20.78	-2.41	7.74	30.00
148	HIS O	-20.87	-3.07	6.68	30.00

Fig. 6B

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
152	CYS N	-12.19	1.21	2.74	30.00
152	CYS CA	-11.12	0.42	2.10	30.00
152	CYS CB	-11.67	-0.96	1.79	30.00
152	CYS SG	-13.13	-0.89	0.76	30.00
152	CYS C	-10.63	1.13	0.86	30.00
152	CYS O	-11.10	2.19	0.50	30.00
156	ARG N	-15.93	-4.07	-3.57	30.00
156	ARG CA	-16.32	-5.09	-4.56	30.00
156	ARG CB	-16.44	-6.44	-3.87	30.00
156	ARG CG	-15.72	-6.48	-2.54	30.00
156	ARG CD	-16.10	-7.68	-1.74	30.00
156	ARG NE	-15.93	-8.92	-2.48	30.00
156	ARG CZ	-15.62	-10.08	-1.91	30.00
156	ARG NH1	-15.48	-11.17	-2.65	30.00
156	ARG NH2	-15.44	-10.16	-0.59	30.00
156	ARG C	-17.57	-4.76	-5.40	30.00
156	ARG O	-17.83	-5.32	-6.46	30.00
157	ARG N	-18.38	-3.86	-4.89	30.00
157	ARG CA	-19.57	-3.45	-5.62	30.00
157	ARG CB	-20.72	-3.30	-4.65	30.00
157	ARG CG	-21.29	-4.64	-4.20	30.00
157	ARG CD	-22.70	-4.56	-3.58	30.00
157	ARG NE	-22.57	-4.44	-2.14	30.00
157	ARG CZ	-22.86	-5.36	-1.23	30.00
157	ARG NH1	-23.39	-6.54	-1.44	30.00
157	ARG NH2	-22.15	-5.29	-0.14	30.00
157	ARG C	-19.22	-2.14	-6.37	30.00
157	ARG O	-18.27	-1.44	-6.03	30.00

Fig. 7A

Figure of the orthogonal three dimensional coordinates in Ångstroms and B factors (\AA^2) for HSV1 protease.

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
15 ALA CB	-3.94	13.47	22.28	30.00
15 ALA C	-4.35	15.65	21.21	30.00
15 ALA O	-3.99	16.48	22.06	30.00
15 ALA N	-2.11	14.64	21.12	30.00
15 ALA CA	-3.54	14.35	21.10	30.00
16 ALA N	-5.16	15.44	20.95	30.00
16 ALA CA	-6.27	15.84	21.83	30.00
16 ALA CB	-5.75	16.59	23.05	30.00
16 ALA C	-7.22	16.78	21.08	30.00
16 ALA O	-6.71	17.71	20.41	30.00
17 ALA N	-8.37	16.64	20.99	30.00
17 ALA CA	-9.22	16.75	19.86	30.00
17 ALA CB	-8.80	18.20	19.75	30.00
17 ALA C	-9.63	16.02	18.57	30.00
17 ALA O	-8.98	16.11	17.52	30.00
18 ALA N	-10.39	14.93	18.74	30.00
18 ALA CA	-10.65	14.73	17.19	30.00
18 ALA CB	-11.47	13.48	17.45	30.00
18 ALA C	-11.39	15.66	16.24	30.00
18 ALA O	-12.13	16.57	16.66	30.00
19 VAL N	-11.08	15.50	14.96	30.00
19 VAL CA	-11.73	16.26	13.87	30.00
19 VAL CB	-10.77	16.47	12.67	30.00
19 VAL CG1	-11.51	17.03	11.45	30.00
19 VAL CG2	-9.67	17.40	13.04	30.00
19 VAL C	-12.85	15.30	13.46	30.00

Fig. 7B

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
19	VAL O	-12.62	14.14	13.13	30.00
20	PRO N	-14.10	15.72	13.65	30.00
20	PRO CD	-14.57	16.88	14.41	30.00
20	PRO CA	-15.21	14.86	13.27	30.00
20	PRO CB	-16.43	15.58	13.85	30.00
20	PRO CG	-15.86	16.35	14.99	30.00
20	PRO C	-15.25	14.87	11.76	30.00
20	PRO O	-15.34	15.91	11.13	30.00
21	ILE N	-15.42	13.51	11.16	30.00
21	ILE CA	-15.27	13.49	9.71	30.00
21	ILE CB	-13.91	12.80	9.34	30.00
21	ILE CG2	-14.13	11.53	8.51	30.00
21	ILE CG1	-12.99	13.77	8.60	30.00
21	ILE CD1	-11.60	13.22	8.35	30.00
21	ILE C	-16.43	12.70	9.11	30.00
21	ILE O	-16.83	11.65	9.61	30.00
22	TYR N	-16.97	13.68	8.21	30.00
22	TYR CA	-18.14	12.98	7.59	30.00
22	TYR CB	-19.26	13.96	7.30	30.00
22	TYR CG	-19.63	14.71	8.49	30.00
22	TYR CD1	-19.94	16.05	8.37	30.00
22	TYR CE1	-20.44	16.76	9.44	30.00
22	TYR CD2	-19.83	14.08	9.71	30.00
22	TYR CE2	-20.33	14.78	10.78	30.00
22	TYR CZ	-20.64	16.12	10.64	30.00
22	TYR OH	-21.16	16.82	11.68	30.00
22	TYR C	-17.68	12.33	6.26	30.00
22	TYR O	-16.91	12.91	5.47	30.00
23	VAL N	-18.49	10.90	6.19	30.00

Fig. 7C

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
23	VAL CA	-18.25	10.08	4.99	30.00
23	VAL CB	-17.91	8.62	5.33	30.00
23	VAL CG1	-16.97	8.01	4.31	30.00
23	VAL CG2	-17.41	8.50	6.71	30.00
23	VAL C	-19.66	10.02	4.39	30.00
23	VAL O	-20.65	9.97	5.11	30.00
24	ALA N	-19.75	9.98	3.08	30.00
24	ALA CA	-21.06	9.90	2.42	30.00
24	ALA CB	-21.59	11.30	2.15	30.00
24	ALA C	-20.75	9.18	1.13	30.00
24	ALA O	-19.65	9.28	0.60	30.00
25	GLY N	-21.70	8.37	0.66	30.00
25	GLY CA	-21.49	7.65	-0.58	30.00
25	GLY C	-22.54	6.57	-0.70	30.00
25	GLY O	-23.32	6.36	0.23	30.00
26	PHE N	-22.73	5.83	-1.73	30.00
26	PHE CA	-23.74	4.80	-1.93	30.00
26	PHE CB	-23.93	4.65	-3.42	30.00
26	PHE CG	-24.81	5.79	-3.94	30.00
26	PHE CD1	-24.23	6.88	-4.59	30.00
26	PHE CD2	-26.17	5.72	-3.79	30.00
26	PHE CE1	-25.06	7.89	-5.08	30.00
26	PHE CE2	-26.99	6.73	-4.29	30.00
26	PHE CZ	-26.41	7.83	-4.94	30.00
26	PHE C	-23.32	3.48	-1.25	30.00
26	PHE O	-22.13	3.10	-1.28	30.00
27	LEU N	-23.57	2.86	-0.72	30.00
27	LEU CA	-23.26	1.51	-0.31	30.00
27	LEU CB	-24.17	1.10	0.83	30.00

Fig. 7D

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
27 LEU CG	-23.69	1.06	2.27	30.00
27 LEU CD1	-23.37	2.44	2.84	30.00
27 LEU CD2	-24.75	0.33	3.02	30.00
27 LEU C	-23.49	0.60	-1.54	30.00
27 LEU O	-22.96	-0.50	-1.65	30.00
28 ALA N	-24.23	0.82	-2.47	30.00
28 ALA CA	-24.47	-0.01	-3.67	30.00
28 ALA CB	-25.14	-1.29	-3.27	30.00
28 ALA C	-25.36	0.76	-4.68	30.00
28 ALA O	-26.14	1.63	-4.32	30.00
29 LEU N	-25.14	0.44	-5.97	30.00
29 LEU CA	-26.00	1.15	-6.96	30.00
29 LEU CB	-25.20	1.58	-8.20	30.00
29 LEU CG	-23.97	2.49	-8.02	30.00
29 LEU CD1	-24.47	3.89	-8.07	30.00
29 LEU CD2	-23.22	2.25	-6.72	30.00
29 LEU C	-27.05	0.10	-7.35	30.00
29 LEU O	-26.73	-1.03	-7.68	30.00
30 TYR N	-28.21	0.18	-7.58	30.00
30 TYR CA	-29.23	-0.80	-7.96	30.00
30 TYR CB	-30.59	-0.15	-7.84	30.00
30 TYR CG	-31.04	0.00	-6.42	30.00
30 TYR CD1	-30.80	-1.01	-5.48	30.00
30 TYR CE1	-31.25	-0.87	-4.19	30.00
30 TYR CD2	-31.74	1.14	-6.00	30.00
30 TYR CE2	-32.19	1.27	-4.71	30.00
30 TYR CZ	-31.94	0.27	-3.82	30.00
30 TYR OH	-32.39	0.40	-2.54	30.00
30 TYR C	-29.14	-1.59	-9.28	30.00

Fig. 7E

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
30 TYR O	-29.28	-2.83	-9.29	30.00
31 ASP N	-28.98	-0.93	-10.42	30.00
31 ASP CA	-28.90	-1.75	-11.66	30.00
31 ASP CB	-30.09	-1.48	-12.60	30.00
31 ASP CG	-31.37	-2.24	-12.19	30.00
31 ASP OD1	-32.44	-1.60	-11.99	30.00
31 ASP OD2	-31.33	-3.49	-12.10	30.00
31 ASP C	-27.57	-1.40	-12.29	30.00
31 ASP O	-27.49	-0.85	-13.39	30.00
32 SER N	-26.52	-1.72	-11.54	30.00
32 SER CA	-25.11	-1.40	-11.94	30.00
32 SER CB	-24.31	-0.92	-10.71	30.00
32 SER OG	-24.43	-1.83	-9.64	30.00
32 SER C	-24.32	-2.51	-12.67	30.00
32 SER O	-23.34	-2.27	-13.38	30.00
33 GLY N	-24.76	-3.74	-12.45	30.00
33 GLY CA	-24.09	-4.86	-13.07	30.00
33 GLY C	-23.28	-5.62	-12.06	30.00
33 GLY O	-22.39	-6.35	-12.46	30.00
34 ASP N	-23.71	-5.38	-10.73	30.00
34 ASP CA	-22.81	-6.14	-9.76	30.00
34 ASP CB	-23.15	-5.87	-8.28	30.00
34 ASP CG	-23.41	-4.40	-7.98	30.00
34 ASP OD1	-23.66	-3.62	-8.93	30.00
34 ASP OD2	-23.39	-4.02	-6.81	30.00
34 ASP C	-23.00	-7.64	-10.05	30.00
34 ASP O	-24.10	-8.09	-10.40	30.00
35 SER N	-22.14	-8.42	-9.62	30.00
35 SER CA	-22.07	-9.88	-9.87	30.00

Fig. 7F

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
35	SER CB	-20.80	-10.44	-9.22	30.00
35	SER OG	-21.23	-11.56	-8.48	30.00
35	SER C	-23.28	-10.61	-9.28	30.00
35	SER O	-24.09	-10.02	-8.51	30.00
36	GLY N	-23.70	-11.73	-9.47	30.00
36	GLY CA	-24.89	-12.34	-8.89	30.00
36	GLY C	-25.04	-12.12	-7.41	30.00
36	GLY O	-25.99	-11.51	-6.95	30.00
37	GLU N	-24.07	-12.51	-6.64	30.00
37	GLU CA	-23.93	-12.42	-5.18	30.00
37	GLU CB	-22.84	-13.41	-4.75	30.00
37	GLU CG	-22.73	-13.63	-3.21	30.00
37	GLU CD	-23.38	-14.91	-2.73	30.00
37	GLU OE1	-23.96	-14.92	-1.62	30.00
37	GLU OE2	-23.32	-15.91	-3.48	30.00
37	GLU C	-23.67	-11.02	-4.56	30.00
37	GLU O	-24.32	-10.58	-3.61	30.00
38	LEU N	-23.20	-10.28	-4.85	30.00
38	LEU CA	-23.10	-8.86	-4.46	30.00
38	LEU CB	-21.80	-8.30	-5.04	30.00
38	LEU CG	-20.54	-8.55	-4.19	30.00
38	LEU CD1	-20.92	-9.02	-2.79	30.00
38	LEU CD2	-19.61	-9.56	-4.88	30.00
38	LEU C	-24.30	-7.95	-4.78	30.00
38	LEU O	-24.58	-6.99	-4.09	30.00
39	ALA N	-24.99	-8.10	-5.82	30.00
39	ALA CA	-26.14	-7.26	-6.20	30.00
39	ALA CB	-26.88	-7.89	-7.37	30.00
39	ALA C	-27.13	-6.99	-5.07	30.00

Fig. 7G

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
39	ALA O	-27.44	-7.83	-4.23	30.00
40	LEU N	-27.69	-5.88	-5.02	30.00
40	LEU CA	-28.65	-5.45	-4.00	30.00
40	LEU CB	-28.07	-4.29	-3.19	30.00
40	LEU CG	-27.45	-4.63	-1.83	30.00
40	LEU CD1	-26.29	-3.67	-1.51	30.00
40	LEU CD2	-28.51	-4.56	-0.76	30.00
40	LEU C	-29.90	-5.03	-4.75	30.00
40	LEU O	-29.85	-4.48	-5.84	30.00
41	ASP N	-31.10	-4.72	-4.25	30.00
41	ASP CA	-32.26	-4.39	-5.09	30.00
41	ASP CB	-32.83	-5.67	-5.67	30.00
41	ASP CG	-32.63	-6.82	-4.76	30.00
41	ASP OD1	-33.63	-7.49	-4.46	30.00
41	ASP OD2	-31.47	-7.03	-4.36	30.00
41	ASP C	-33.31	-3.57	-4.33	30.00
41	ASP O	-33.35	-3.56	-3.12	30.00
42	PRO N	-33.98	-2.73	-4.64	30.00
42	PRO CD	-34.24	-2.52	-6.07	30.00
42	PRO CA	-34.86	-1.88	-3.84	30.00
42	PRO CB	-35.77	-1.27	-4.90	30.00
42	PRO CG	-34.93	-1.18	-6.04	30.00
42	PRO C	-35.65	-2.54	-2.74	30.00
42	PRO O	-35.66	-2.10	-1.59	30.00
43	ASP N	-36.49	-3.44	-3.10	30.00
43	ASP CA	-37.09	-4.30	-2.07	30.00
43	ASP CB	-37.91	-5.36	-2.72	30.00
43	ASP CG	-38.97	-4.78	-3.62	30.00
43	ASP OD1	-39.44	-3.64	-3.38	30.00

Fig. 7H

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
43	ASP OD2	-39.34	-5.47	-4.56	30.00
43	ASP C	-36.10	-4.90	-1.07	30.00
43	ASP O	-36.40	-5.03	0.10	30.00
44	THR N	-35.16	-5.37	-1.04	30.00
44	THR CA	-34.25	-5.88	-0.01	30.00
44	THR CB	-33.30	-6.88	-0.61	30.00
44	THR OG1	-33.56	-8.11	0.04	30.00
44	THR CG2	-31.84	-6.49	-0.34	30.00
44	THR C	-33.47	-4.73	0.66	30.00
44	THR O	-33.11	-4.78	1.83	30.00
45	VAL N	-33.47	-3.66	0.15	30.00
45	VAL CA	-32.95	-2.57	0.94	30.00
45	VAL CB	-32.35	-1.49	0.10	30.00
45	VAL CG1	-33.00	-0.16	0.42	30.00
45	VAL CG2	-30.88	-1.40	0.39	30.00
45	VAL C	-34.09	-2.03	1.78	30.00
45	VAL O	-33.95	-1.74	2.97	30.00
46	ARG N	-35.27	-1.97	1.18	30.00
46	ARG CA	-36.46	-1.46	1.86	30.00
46	ARG CB	-37.68	-1.61	0.95	30.00
46	ARG CG	-38.95	-0.93	1.45	30.00
46	ARG CD	-38.82	0.62	1.44	30.00
46	ARG NE	-37.98	1.15	2.54	30.00
46	ARG CZ	-37.83	2.44	2.87	30.00
46	ARG NH1	-37.05	2.76	3.90	30.00
46	ARG NH2	-38.46	3.40	2.19	30.00
46	ARG C	-36.68	-2.22	3.15	30.00
46	ARG O	-36.92	-1.68	4.21	30.00
47	ALA N	-36.53	-3.53	3.06	30.00

Fig. 7I

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
47 ALA CA	-36.72	-4.42	4.21	30.00
47 ALA CB	-36.90	-5.83	3.70	30.00
47 ALA C	-35.59	-4.37	5.27	30.00
47 ALA O	-35.71	-4.91	6.36	30.00
48 ALA N	-34.48	-3.73	4.95	30.00
48 ALA CA	-33.35	-3.67	5.88	30.00
48 ALA CB	-32.07	-3.88	5.13	30.00
48 ALA C	-33.32	-2.34	6.62	30.00
48 ALA O	-32.55	-2.13	7.55	30.00
49 LEU N	-34.00	-1.44	6.23	30.00
49 LEU CA	-34.13	-0.13	6.85	30.00
49 LEU CB	-34.20	0.93	5.74	30.00
49 LEU CG	-32.85	1.45	5.22	30.00
49 LEU CD1	-31.95	0.27	4.91	30.00
49 LEU CD2	-33.03	2.37	4.00	30.00
49 LEU C	-35.33	-0.01	7.79	30.00
49 LEU O	-36.43	-0.46	7.49	30.00
50 PRO N	-35.21	0.72	8.93	30.00
50 PRO CD	-36.32	1.15	9.78	30.00
50 PRO CA	-33.93	1.16	9.51	30.00
50 PRO CB	-34.37	2.00	10.71	30.00
50 PRO CG	-35.75	2.40	10.37	30.00
50 PRO C	-33.19	-0.05	10.02	30.00
50 PRO O	-33.77	-1.09	10.30	30.00
51 PRO N	-31.86	0.07	10.13	30.00
51 PRO CD	-30.97	1.13	9.63	30.00
51 PRO CA	-31.11	-1.08	10.61	30.00
51 PRO CB	-29.66	-0.59	10.52	30.00
51 PRO CG	-29.71	0.37	9.35	30.00

Fig. 7J

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
51 PRO C	-31.52	-1.42	12.06	30.00
51 PRO O	-31.80	-0.55	12.86	30.00
52 ASP N	-31.64	-2.67	12.33	30.00
52 ASP CA	-31.97	-3.14	13.66	30.00
52 ASP CB	-31.91	-4.64	13.83	30.00
52 ASP CG	-30.69	-5.08	14.67	30.00
52 ASP OD1	-29.91	-5.96	14.24	30.00
52 ASP OD2	-30.54	-4.51	15.77	30.00
52 ASP C	-30.99	-2.61	14.69	30.00
52 ASP O	-31.28	-1.86	15.70	30.00
53 ASN N	-29.69	-2.75	14.39	30.00
53 ASN CA	-28.61	-2.21	15.22	30.00
53 ASN CB	-27.80	-3.36	15.82	30.00
53 ASN CG	-28.50	-4.01	17.00	30.00
53 ASN OD1	-28.90	-5.17	16.94	30.00
53 ASN ND2	-28.67	-3.25	18.09	30.00
53 ASN C	-27.73	-1.24	14.43	30.00
53 ASN O	-27.63	-1.33	13.21	30.00
54 PRO N	-27.11	-0.28	15.13	30.00
54 PRO CD	-27.15	-0.08	16.59	30.00
54 PRO CA	-26.25	0.72	14.51	30.00
54 PRO CB	-25.66	1.47	15.71	30.00
54 PRO CG	-26.76	1.38	16.73	30.00
54 PRO C	-25.16	0.07	13.69	30.00
54 PRO O	-24.69	-1.02	13.97	30.00
55 LEU N	-24.80	0.75	12.62	30.00
55 LEU CA	-23.78	0.22	11.77	30.00
55 LEU CB	-24.11	0.42	10.30	30.00
55 LEU CG	-25.51	0.00	9.89	30.00

Fig. 7K

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
55	LEU CD1	-25.88	0.69	8.61	30.00
55	LEU CD2	-25.53	-1.47	9.70	30.00
55	LEU C	-22.51	0.92	12.12	30.00
55	LEU O	-22.39	2.13	12.02	30.00
56	PRO N	-21.57	0.19	12.69	30.00
56	PRO CD	-21.73	-1.18	13.22	30.00
56	PRO CA	-20.28	0.75	13.06	30.00
56	PRO CB	-19.68	-0.37	13.89	30.00
56	PRO CG	-20.33	-1.60	13.32	30.00
56	PRO C	-19.47	0.92	11.77	30.00
56	PRO O	-19.78	0.31	10.74	30.00
57	ILE N	-18.43	1.76	11.81	30.00
57	ILE CA	-17.58	1.93	10.62	30.00
57	ILE CB	-17.48	3.40	10.17	30.00
57	ILE CG2	-16.33	3.57	9.12	30.00
57	ILE CG1	-18.84	3.89	9.64	30.00
57	ILE CD1	-18.86	5.33	9.33	30.00
57	ILE C	-16.20	1.48	11.04	30.00
57	ILE O	-15.67	1.92	12.06	30.00
58	ASN N	-15.65	0.54	10.30	30.00
58	ASN CA	-14.31	0.08	10.61	30.00
58	ASN CB	-14.34	-1.30	11.24	30.00
58	ASN CG	-15.14	-2.27	10.45	30.00
58	ASN OD1	-15.41	-2.06	9.29	30.00
58	ASN ND2	-15.47	-3.39	11.08	30.00
58	ASN C	-13.40	0.16	9.39	30.00
58	ASN O	-13.83	0.51	8.31	30.00
59	VAL N	-12.10	-0.06	9.60	30.00
59	VAL CA	-11.13	0.02	8.50	30.00

Fig. 7L

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
59 VAL CB	-9.80	0.66	8.94	30.00
59 VAL CG1	-8.68	-0.36	8.84	30.00
59 VAL CG2	-9.46	1.85	8.06	30.00
59 VAL C	-10.84	-1.36	7.96	30.00
59 VAL O	-10.50	-2.28	8.69	30.00
60 ASP N	-11.00	-1.52	6.66	30.00
60 ASP CA	-10.72	-2.81	5.98	30.00
60 ASP CB	-9.21	-2.88	5.67	30.00
60 ASP CG	-8.78	-4.21	5.06	30.00
60 ASP OD1	-9.01	-4.42	3.83	30.00
60 ASP OD2	-8.20	-5.04	5.80	30.00
60 ASP C	-11.21	-4.08	6.77	30.00
60 ASP O	-10.44	-4.98	7.14	30.00
61 HIS N	-12.45	-4.14	6.98	30.00
61 HIS CA	-13.09	-5.29	7.68	30.00
61 HIS CB	-13.58	-6.34	6.67	30.00
61 HIS CG	-14.61	-5.80	5.72	30.00
61 HIS CD2	-14.77	-4.58	5.17	30.00
61 HIS ND1	-15.59	-6.59	5.17	30.00
61 HIS CE1	-16.31	-5.88	4.32	30.00
61 HIS NE2	-15.84	-4.65	4.30	30.00
61 HIS C	-12.35	-5.97	8.84	30.00
61 HIS O	-12.85	-6.93	9.45	30.00
62 ARG N	-11.45	-5.26	9.41	30.00
62 ARG CA	-10.77	-5.67	10.63	30.00
62 ARG CB	-9.40	-4.99	10.64	30.00
62 ARG CG	-8.40	-5.55	9.64	30.00
62 ARG CD	-8.02	-6.99	10.03	30.00
62 ARG NE	-7.41	-7.05	11.36	30.00

Fig. 7M

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
62	ARG CZ	-6.11	-7.26	11.59	30.00
62	ARG NH1	-5.28	-7.45	10.57	30.00
62	ARG NH2	-5.66	-7.28	12.84	30.00
62	ARG C	-11.72	-5.10	11.71	30.00
62	ARG O	-11.66	-3.91	12.06	30.00
63	ALA N	-12.65	-5.94	12.17	30.00
63	ALA CA	-13.67	-5.52	13.18	30.00
63	ALA CB	-14.63	-6.65	13.48	30.00
63	ALA C	-13.13	-4.90	14.48	30.00
63	ALA O	-13.87	-4.36	15.29	30.00
64	GLY N	-11.80	-5.03	14.74	30.00
64	GLY CA	-11.16	-4.41	15.87	30.00
64	GLY C	-11.01	-2.93	15.71	30.00
64	GLY O	-11.01	-2.10	16.66	30.00
65	CYS N	-10.97	-2.54	14.41	30.00
65	CYS CA	-10.80	-1.13	13.96	30.00
65	CYS CB	-10.05	-1.10	12.66	30.00
65	CYS SG	-8.41	-0.83	12.94	30.00
65	CYS C	-12.03	-0.29	13.80	30.00
65	CYS O	-12.26	0.29	12.76	30.00
66	GLU N	-12.83	-0.02	14.72	30.00
66	GLU CA	-14.08	0.65	14.67	30.00
66	GLU CB	-14.86	0.23	15.88	30.00
66	GLU CG	-16.24	0.71	15.83	30.00
66	GLU CD	-17.02	0.26	17.00	30.00
66	GLU OE1	-16.95	-0.95	17.33	30.00
66	GLU OE2	-17.71	1.11	17.59	30.00
66	GLU C	-13.70	2.13	14.62	30.00
66	GLU O	-12.85	2.58	15.40	30.00

Fig. 7N

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
67 VAL N	-13.84	2.95	14.01	30.00
67 VAL CA	-13.40	4.36	14.03	30.00
67 VAL CB	-12.41	4.67	12.88	30.00
67 VAL CG1	-11.69	3.38	12.41	30.00
67 VAL CG2	-13.14	5.34	11.72	30.00
67 VAL C	-14.59	5.34	13.93	30.00
67 VAL O	-14.46	6.57	14.03	30.00
68 GLY N	-15.78	4.79	13.74	30.00
68 GLY CA	-16.94	5.64	13.61	30.00
68 GLY C	-18.27	4.91	13.65	30.00
68 GLY O	-18.34	3.73	14.03	30.00
69 ARG N	-19.32	5.62	13.23	30.00
69 ARG CA	-20.69	5.08	13.24	30.00
69 ARG CB	-21.30	5.44	14.59	30.00
69 ARG CG	-22.72	5.00	14.79	30.00
69 ARG CD	-22.78	3.52	14.82	30.00
69 ARG NE	-22.16	2.94	16.01	30.00
69 ARG CZ	-22.59	3.15	17.25	30.00
69 ARG NH1	-21.97	2.54	18.26	30.00
69 ARG NH2	-23.59	3.98	17.50	30.00
69 ARG C	-21.52	5.67	12.09	30.00
69 ARG O	-21.52	6.88	11.82	30.00
70 VAL N	-22.20	4.78	11.37	30.00
70 VAL CA	-23.09	5.14	10.27	30.00
70 VAL CB	-23.62	3.87	9.58	30.00
70 VAL CG1	-24.86	4.18	8.76	30.00
70 VAL CG2	-22.54	3.25	8.72	30.00
70 VAL C	-24.30	5.91	10.89	30.00
70 VAL O	-25.06	5.36	11.70	30.00

Fig. 70

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
71 LEU N	-24.43	7.18	10.54	30.00
71 LEU CA	-25.56	8.01	11.06	30.00
71 LEU CB	-25.22	9.48	10.94	30.00
71 LEU CG	-24.36	10.11	11.99	30.00
71 LEU CD1	-23.36	9.11	12.48	30.00
71 LEU CD2	-23.72	11.34	11.44	30.00
71 LEU C	-26.95	7.73	10.37	30.00
71 LEU O	-28.00	7.65	11.04	30.00
72 ALA N	-27.07	7.71	9.08	30.00
72 ALA CA	-28.21	7.52	8.18	30.00
72 ALA CB	-28.67	8.84	7.64	30.00
72 ALA C	-27.92	6.60	7.01	30.00
72 ALA O	-26.86	6.58	6.42	30.00
73 VAL N	-28.88	5.80	6.62	30.00
73 VAL CA	-28.88	5.00	5.38	30.00
73 VAL CB	-28.79	3.51	5.66	30.00
73 VAL CG1	-28.66	2.73	4.36	30.00
73 VAL CG2	-27.61	3.23	6.54	30.00
73 VAL C	-30.25	5.30	4.77	30.00
73 VAL O	-31.27	5.07	5.38	30.00
74 VAL N	-30.27	5.92	3.55	30.00
74 VAL CA	-31.56	6.30	3.00	30.00
74 VAL CB	-31.60	7.78	2.65	30.00
74 VAL CG1	-32.95	8.12	2.08	30.00
74 VAL CG2	-31.35	8.62	3.87	30.00
74 VAL C	-31.84	5.48	1.74	30.00
74 VAL O	-30.99	5.31	0.85	30.00
75 ASP N	-32.72	4.94	1.33	30.00
75 ASP CA	-32.92	4.24	0.08	30.00

Fig. 7P

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
75 ASP CB	-34.07	3.26	0.08	30.00
75 ASP CG	-35.35	3.87	-0.53	30.00
75 ASP OD1	-35.40	4.16	-1.75	30.00
75 ASP OD2	-36.31	4.04	0.24	30.00
75 ASP C	-33.26	5.20	-1.05	30.00
75 ASP O	-34.28	5.88	-1.16	30.00
76 ASP N	-32.19	5.56	-1.85	30.00
76 ASP CA	-32.32	6.53	-2.92	30.00
76 ASP CB	-30.99	7.21	-3.15	30.00
76 ASP CG	-31.14	8.53	-3.80	30.00
76 ASP OD1	-32.27	9.05	-3.91	30.00
76 ASP OD2	-30.13	9.10	-4.18	30.00
76 ASP C	-32.72	5.74	-4.16	30.00
76 ASP O	-32.37	4.55	-4.29	30.00
77 PRO N	-33.44	6.38	-5.10	30.00
77 PRO CD	-34.03	7.73	-5.05	30.00
77 PRO CA	-33.85	5.70	-6.32	30.00
77 PRO CB	-34.39	6.84	-7.17	30.00
77 PRO CG	-35.00	7.72	-6.20	30.00
77 PRO C	-32.68	4.99	-7.04	30.00
77 PRO O	-32.86	4.08	-7.82	30.00
78 ARG N	-31.46	5.42	-6.73	30.00
78 ARG CA	-30.27	4.82	-7.34	30.00
78 ARG CB	-29.29	5.93	-7.65	30.00
78 ARG CG	-29.81	7.03	-8.57	30.00
78 ARG CD	-28.72	8.08	-8.86	30.00
78 ARG NE	-27.54	7.46	-9.50	30.00
78 ARG CZ	-26.27	7.78	-9.27	30.00
78 ARG NH1	-25.31	7.13	-9.93	30.00

Fig. 7Q

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
78 ARG NH2	-25.93	8.71	-8.37	30.00
78 ARG C	-29.59	3.70	-6.48	30.00
78 ARG O	-28.91	2.81	-6.99	30.00
79 GLY N	-29.82	3.73	-5.18	30.00
79 GLY CA	-29.20	2.73	-4.33	30.00
79 GLY C	-29.17	3.22	-2.91	30.00
79 GLY O	-29.45	4.39	-2.64	30.00
80 PRO N	-28.81	2.36	-1.96	30.00
80 PRO CD	-28.38	0.96	-2.15	30.00
80 PRO CA	-28.75	2.75	-0.56	30.00
80 PRO CB	-28.49	1.43	0.16	30.00
80 PRO CG	-27.68	0.65	-0.81	30.00
80 PRO C	-27.59	3.69	-0.36	30.00
80 PRO O	-26.43	3.33	-0.57	30.00
81 PHE N	-27.92	4.90	0.02	30.00
81 PHE CA	-26.95	5.96	0.30	30.00
81 PHE CB	-27.46	7.23	-0.34	30.00
81 PHE CG	-26.34	8.26	-0.42	30.00
81 PHE CD1	-26.60	9.51	-0.97	30.00
81 PHE CD2	-25.10	7.94	0.05	30.00
81 PHE CE1	-25.55	10.44	-1.01	30.00
81 PHE CE2	-24.07	8.87	0.01	30.00
81 PHE CZ	-24.32	10.14	-0.53	30.00
81 PHE C	-26.73	6.11	1.81	30.00
81 PHE O	-27.70	5.95	2.56	30.00
82 PHE N	-25.51	6.37	2.30	30.00
82 PHE CA	-25.35	6.50	3.75	30.00
82 PHE CB	-24.74	5.22	4.25	30.00
82 PHE CG	-23.22	5.28	4.13	30.00

Fig. 7R

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
82	PHE CD1	-22.48	4.10	4.12	30.00
82	PHE CD2	-22.60	6.49	4.01	30.00
82	PHE CE1	-21.09	4.19	3.98	30.00
82	PHE CE2	-21.23	6.57	3.86	30.00
82	PHE CZ	-20.47	5.39	3.85	30.00
82	PHE C	-24.49	7.73	4.08	30.00
82	PHE O	-23.75	8.29	3.30	30.00
83	VAL N	-24.58	8.09	5.37	30.00
83	VAL CA	-23.77	9.17	5.91	30.00
83	VAL CB	-24.57	10.41	6.07	30.00
83	VAL CG1	-23.82	11.39	6.92	30.00
83	VAL CG2	-24.82	11.01	4.70	30.00
83	VAL C	-23.25	8.70	7.26	30.00
83	VAL O	-23.99	8.27	8.13	30.00
84	GLY N	-21.92	8.75	7.40	30.00
84	GLY CA	-21.27	8.34	8.62	30.00
84	GLY C	-20.40	9.39	9.27	30.00
84	GLY O	-20.10	10.43	8.69	30.00
85	LEU N	-19.80	9.19	10.33	30.00
85	LEU CA	-19.06	10.04	11.27	30.00
85	LEU CB	-20.00	10.54	12.38	30.00
85	LEU CG	-19.83	12.01	12.82	30.00
85	LEU CD1	-18.67	12.22	13.79	30.00
85	LEU CD2	-19.63	12.86	11.59	30.00
85	LEU C	-17.89	9.27	11.87	30.00
85	LEU O	-18.04	8.19	12.42	30.00
86	ILE N	-16.79	9.78	11.64	30.00
86	ILE CA	-15.53	9.18	12.07	30.00
86	ILE CB	-14.63	9.04	10.85	30.00

Fig. 7S

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
86	ILE CG2	-13.21	8.65	11.22	30.00
86	ILE CG1	-15.28	8.06	9.88	30.00
86	ILE CD1	-14.81	8.24	8.47	30.00
86	ILE C	-14.94	10.17	13.07	30.00
86	ILE O	-14.65	11.33	12.75	30.00
87	ALA N	-14.83	9.75	14.31	30.00
87	ALA CA	-14.26	10.62	15.36	30.00
87	ALA CB	-15.31	10.96	16.38	30.00
87	ALA C	-13.15	9.75	15.96	30.00
87	ALA O	-13.35	8.98	16.90	30.00
88	CYS N	-12.03	9.67	15.53	30.00
88	CYS CA	-10.79	8.98	15.81	30.00
88	CYS CB	-10.71	7.77	14.93	30.00
88	CYS SG	-9.21	6.86	15.04	30.00
88	CYS C	-9.63	9.91	15.52	30.00
88	CYS O	-9.37	10.26	14.37	30.00
89	VAL N	-8.92	10.28	16.53	30.00
89	VAL CA	-7.60	10.92	16.48	30.00
89	VAL CB	-7.43	11.79	17.71	30.00
89	VAL CG1	-7.34	10.94	18.99	30.00
89	VAL CG2	-6.22	12.64	17.53	30.00
89	VAL C	-6.45	9.91	16.38	30.00
89	VAL O	-5.41	10.16	15.78	30.00
90	GLN N	-6.48	8.80	16.66	30.00
90	GLN CA	-5.36	7.87	16.41	30.00
90	GLN CB	-5.54	6.58	17.23	30.00
90	GLN CG	-5.90	6.86	18.66	30.00
90	GLN CD	-6.38	5.63	19.39	30.00
90	GLN OE1	-5.74	4.60	19.38	30.00

Fig. 7T

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
90 GLN NE2	-7.52	5.74	20.02	30.00
90 GLN C	-5.25	7.56	14.91	30.00
90 GLN O	-4.17	7.48	14.33	30.00
91 LEU N	-6.49	7.40	14.26	30.00
91 LEU CA	-6.45	7.38	12.78	30.00
91 LEU CB	-7.85	7.13	12.28	30.00
91 LEU CG	-8.16	7.42	10.81	30.00
91 LEU CD1	-8.78	6.21	10.14	30.00
91 LEU CD2	-9.06	8.62	10.75	30.00
91 LEU C	-5.90	8.76	12.31	30.00
91 LEU O	-5.12	8.84	11.37	30.00
92 GLU N	-6.04	9.82	12.69	30.00
92 GLU CA	-5.47	11.12	12.24	30.00
92 GLU CB	-5.94	12.28	13.13	30.00
92 GLU CG	-7.00	13.13	12.51	30.00
92 GLU CD	-7.00	14.55	13.05	30.00
92 GLU OE1	-8.01	14.92	13.71	30.00
92 GLU OE2	-6.02	15.29	12.78	30.00
92 GLU C	-3.96	11.09	12.30	30.00
92 GLU O	-3.28	11.29	11.31	30.00
93 ARG N	-3.44	10.86	13.51	30.00
93 ARG CA	-1.99	10.79	13.77	30.00
93 ARG CB	-1.75	10.54	15.25	30.00
93 ARG CG	-1.15	11.73	15.96	30.00
93 ARG CD	-2.06	12.97	15.97	30.00
93 ARG NE	-1.83	13.75	17.20	30.00
93 ARG CZ	-2.34	14.96	17.45	30.00
93 ARG NH1	-2.05	15.57	18.61	30.00
93 ARG NH2	-3.13	15.56	16.57	30.00

Fig. 7U

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
93 ARG C	-1.25	9.77	12.93	30.00
93 ARG O	-0.27	10.08	12.27	30.00
94 VAL N	-1.73	8.57	12.87	30.00
94 VAL CA	-1.10	7.44	12.13	30.00
94 VAL CB	-1.84	6.11	12.44	30.00
94 VAL CG1	-1.51	5.08	11.45	30.00
94 VAL CG2	-1.51	5.64	13.83	30.00
94 VAL C	-1.11	7.70	10.59	30.00
94 VAL O	-0.13	7.48	9.91	30.00
95 LEU N	-2.03	8.16	10.10	30.00
95 LEU CA	-1.95	8.81	8.73	30.00
95 LEU CB	-3.32	9.37	8.34	30.00
95 LEU CG	-4.45	8.51	7.74	30.00
95 LEU CD1	-5.01	9.07	6.42	30.00
95 LEU CD2	-3.92	7.09	7.55	30.00
95 LEU C	-0.88	9.94	8.73	30.00
95 LEU O	-0.01	10.01	7.89	30.00
96 GLU N	-1.20	11.17	9.39	30.00
96 GLU CA	-0.39	12.42	9.42	30.00
96 GLU CB	-0.79	13.31	10.61	30.00
96 GLU CG	-2.07	14.12	10.46	30.00
96 GLU CD	-1.87	15.63	10.67	30.00
96 GLU OE1	-2.70	16.25	11.39	30.00
96 GLU OE2	-0.88	16.19	10.13	30.00
96 GLU C	1.12	12.16	9.52	30.00
96 GLU O	1.95	12.88	8.96	30.00
97 THR N	1.58	11.16	10.05	30.00
97 THR CA	2.95	10.85	10.42	30.00
97 THR CB	3.08	10.38	11.96	30.00

Fig. 7V

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
97 THR OG1	3.73	9.09	12.05	30.00
97 THR CG2	1.72	10.24	12.60	30.00
97 THR C	3.60	9.83	9.46	30.00
97 THR O	4.80	9.83	9.23	30.00
98 ALA N	2.61	9.14	8.82	30.00
98 ALA CA	3.06	8.24	7.73	30.00
98 ALA CB	1.97	7.23	7.38	30.00
98 ALA C	3.38	9.10	6.53	30.00
98 ALA O	4.33	8.92	5.83	30.00
99 ALA N	2.52	10.08	6.31	30.00
99 ALA CA	2.69	10.98	5.20	30.00
99 ALA CB	1.48	11.91	5.09	30.00
99 ALA C	3.94	11.80	5.41	30.00
99 ALA O	3.96	12.79	6.13	30.00
100 SER N	5.01	11.57	4.38	30.00
100 SER CA	6.31	12.16	4.85	30.00
100 SER CB	7.29	11.04	5.23	30.00
100 SER OG	6.80	10.24	6.31	30.00
100 SER C	6.63	13.02	3.69	30.00
100 SER O	7.73	12.73	2.90	30.00
101 ALA N	5.73	13.72	3.16	30.00
101 ALA CA	5.75	14.49	1.94	30.00
101 ALA CB	4.44	15.26	1.77	30.00
101 ALA C	6.93	15.39	1.68	30.00
101 ALA O	7.46	16.12	2.53	30.00
111 ALA N	-0.35	22.93	2.59	30.00
111 ALA CA	-1.80	22.98	2.21	30.00
111 ALA CB	-2.37	21.55	2.11	30.00
111 ALA C	-2.45	23.81	3.33	30.00

Fig. 7W

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
111 ALA O	-2.29	25.04	3.40	30.00
112 SER N	-3.13	23.13	4.25	30.00
112 SER CA	-3.75	23.84	5.36	30.00
112 SER CB	-5.17	24.27	5.01	30.00
112 SER OG	-5.13	25.30	4.03	30.00
112 SER C	-3.71	23.17	6.72	30.00
112 SER O	-2.88	23.50	7.55	30.00
113 ARG N	-4.54	22.16	6.92	30.00
113 ARG CA	-4.61	21.54	8.25	30.00
113 ARG CB	-5.27	22.59	9.11	30.00
113 ARG CG	-6.24	23.49	8.30	30.00
113 ARG CD	-7.34	24.06	9.16	30.00
113 ARG NE	-6.84	24.47	10.48	30.00
113 ARG CZ	-6.78	23.66	11.54	30.00
113 ARG NH1	-6.30	24.12	12.70	30.00
113 ARG NH2	-7.19	22.40	11.46	30.00
113 ARG C	-5.39	20.21	8.27	30.00
113 ARG O	-4.91	19.14	7.92	30.00
114 GLU N	-6.63	20.28	8.74	30.00
114 GLU CA	-7.49	19.10	8.72	30.00
114 GLU CB	-8.78	19.37	9.50	30.00
114 GLU CG	-8.70	20.45	10.56	30.00
114 GLU CD	-9.85	21.46	10.51	30.00
114 GLU OE1	-11.04	21.05	10.53	30.00
114 GLU OE2	-9.57	22.67	10.44	30.00
114 GLU C	-7.77	18.75	7.22	30.00
114 GLU O	-8.22	17.66	6.88	30.00
115 GLU N	-7.45	19.88	6.38	30.00
115 GLU CA	-7.54	19.49	4.96	30.00

Fig. 7X

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
115 GLU CB	-7.57	20.74	4.08	30.00
115 GLU CG	-6.19	21.06	3.51	30.00
115 GLU CD	-6.17	22.26	2.57	30.00
115 GLU OE1	-5.39	22.25	1.59	30.00
115 GLU OE2	-6.97	23.20	2.80	30.00
115 GLU C	-6.35	18.58	4.66	30.00
115 GLU O	-6.43	17.61	3.91	30.00
116 ARG N	-5.40	18.59	5.09	30.00
116 ARG CA	-4.29	17.67	4.84	30.00
116 ARG CB	-3.10	18.09	5.70	30.00
116 ARG CG	-1.93	17.09	5.76	30.00
116 ARG CD	-0.53	17.79	5.75	30.00
116 ARG NE	-0.05	17.96	4.38	30.00
116 ARG CZ	0.96	17.29	3.82	30.00
116 ARG NH1	1.68	16.41	4.50	30.00
116 ARG NH2	1.09	17.34	2.51	30.00
116 ARG C	-4.82	16.28	5.25	30.00
116 ARG O	-4.58	15.26	4.63	30.00
117 LEU N	-5.59	16.27	6.32	30.00
117 LEU CA	-6.17	15.04	6.81	30.00
117 LEU CB	-6.78	15.27	8.18	30.00
117 LEU CG	-7.67	14.15	8.74	30.00
117 LEU CD1	-6.97	12.80	8.72	30.00
117 LEU CD2	-8.08	14.53	10.14	30.00
117 LEU C	-7.20	14.54	5.83	30.00
117 LEU O	-7.26	13.35	5.50	30.00
118 LEU N	-8.03	15.46	5.33	30.00
118 LEU CA	-9.11	15.10	4.34	30.00
118 LEU CB	-9.96	16.30	4.00	30.00

Fig. 7Y

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
118 LEU CG	-11.29	16.41	4.74	30.00
118 LEU CD1	-11.56	15.18	5.59	30.00
118 LEU CD2	-11.27	17.66	5.53	30.00
118 LEU C	-8.49	14.52	3.08	30.00
118 LEU O	-8.90	13.47	2.57	30.00
119 TYR N	-7.29	15.04	2.80	30.00
119 TYR CA	-6.59	14.64	1.58	30.00
119 TYR CB	-5.67	15.78	1.09	30.00
119 TYR CG	-4.59	15.32	0.15	30.00
119 TYR CD1	-4.63	15.66	-1.21	30.00
119 TYR CE1	-3.63	15.29	-2.08	30.00
119 TYR CD2	-3.51	14.57	0.63	30.00
119 TYR CE2	-2.50	14.18	-0.24	30.00
119 TYR CZ	-2.57	14.55	-1.59	30.00
119 TYR OH	-1.56	14.22	-2.46	30.00
119 TYR C	-5.82	13.34	1.83	30.00
119 TYR O	-5.84	12.40	1.03	30.00
120 LEU N	-5.50	13.19	2.83	30.00
120 LEU CA	-4.86	11.88	3.18	30.00
120 LEU CB	-4.07	12.05	4.47	30.00
120 LEU CG	-2.57	12.37	4.51	30.00
120 LEU CD1	-1.70	11.14	4.50	30.00
120 LEU CD2	-2.25	13.27	3.34	30.00
120 LEU C	-5.87	10.72	3.28	30.00
120 LEU O	-5.68	9.66	2.68	30.00
121 ILE N	-6.91	10.75	3.95	30.00
121 ILE CA	-7.98	9.72	4.07	30.00
121 ILE CB	-8.79	9.85	5.41	30.00
121 ILE CG2	-9.51	11.15	5.51	30.00

Fig. 7Z

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
121	ILE CG1	-9.83	8.74	5.47	30.00
121	ILE CD1	-10.35	8.51	6.84	30.00
121	ILE C	-8.90	9.61	2.82	30.00
121	ILE O	-9.20	8.51	2.35	30.00
122	THR N	-9.10	10.50	2.10	30.00
122	THR CA	-9.83	10.33	0.82	30.00
122	THR CB	-10.07	11.65	0.14	30.00
122	THR OG1	-10.72	12.53	1.05	30.00
122	THR CG2	-10.96	11.44	-1.06	30.00
122	THR C	-9.12	9.48	-0.22	30.00
122	THR O	-9.69	8.57	-0.84	30.00
123	ASN N	-7.87	9.83	-0.48	30.00
123	ASN CA	-7.07	9.10	-1.48	30.00
123	ASN CB	-5.96	9.99	-1.98	30.00
123	ASN CG	-6.48	11.26	-2.63	30.00
123	ASN OD1	-6.43	12.34	-2.05	30.00
123	ASN ND2	-7.03	11.13	-3.81	30.00
123	ASN C	-6.54	7.76	-1.01	30.00
123	ASN O	-6.25	6.89	-1.81	30.00
124	PHE N	-6.37	7.56	0.36	30.00
124	PHE CA	-5.94	6.25	0.83	30.00
124	PHE CB	-5.24	6.45	2.16	30.00
124	PHE CG	-4.44	5.20	2.52	30.00
124	PHE CD1	-5.10	4.04	2.87	30.00
124	PHE CD2	-3.07	5.24	2.48	30.00
124	PHE CE1	-4.34	2.90	3.17	30.00
124	PHE CE2	-2.33	4.12	2.78	30.00
124	PHE CZ	-2.98	2.93	3.12	30.00
124	PHE C	-7.14	5.30	0.95	30.00

Fig. 7AA

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
124 PHE O	-7.07	4.15	0.63	30.00
125 LEU N	-8.08	5.73	1.56	30.00
125 LEU CA	-9.32	4.99	1.69	30.00
125 LEU CB	-9.77	5.01	3.15	30.00
125 LEU CG	-8.88	4.23	4.14	30.00
125 LEU CD1	-9.27	2.78	4.09	30.00
125 LEU CD2	-7.39	4.39	3.83	30.00
125 LEU C	-10.41	5.55	0.74	30.00
125 LEU O	-11.43	6.09	1.17	30.00
126 PRO N	-10.55	5.54	-0.42	30.00
126 PRO CD	-9.43	5.04	-1.24	30.00
126 PRO CA	-11.63	6.07	-1.27	30.00
126 PRO CB	-10.92	6.24	-2.62	30.00
126 PRO CG	-9.94	5.12	-2.64	30.00
126 PRO C	-12.97	5.29	-1.41	30.00
126 PRO O	-13.97	5.86	-1.87	30.00
127 SER N	-13.02	4.04	-0.93	30.00
127 SER CA	-14.26	3.19	-1.03	30.00
127 SER CB	-13.93	1.96	-1.87	30.00
127 SER OG	-13.37	2.32	-3.11	30.00
127 SER C	-14.96	2.72	0.26	30.00
127 SER O	-14.42	2.75	1.36	30.00
128 VAL N	-16.20	2.27	0.10	30.00
128 VAL CA	-16.96	1.68	1.24	30.00
128 VAL CB	-18.36	2.23	1.51	30.00
128 VAL CG1	-18.31	3.21	2.64	30.00
128 VAL CG2	-18.97	2.80	0.28	30.00
128 VAL C	-17.24	0.27	0.83	30.00
128 VAL O	-17.25	-0.10	-0.33	30.00

Fig. 7BB

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
129	SER N	-17.57	-0.53	1.82	30.00
129	SER CA	-17.87	-1.90	1.55	30.00
129	SER CB	-16.59	-2.67	1.72	30.00
129	SER OG	-16.86	-4.06	1.63	30.00
129	SER C	-18.86	-2.27	2.69	30.00
129	SER O	-18.55	-2.30	3.78	30.00
130	LEU N	-19.99	-2.64	2.45	30.00
130	LEU CA	-21.21	-2.90	3.21	30.00
130	LEU CB	-22.45	-2.72	2.32	30.00
130	LEU CG	-23.71	-2.26	3.04	30.00
130	LEU CD1	-24.41	-1.17	2.24	30.00
130	LEU CD2	-24.61	-3.49	3.20	30.00
130	LEU C	-21.18	-4.29	3.74	30.00
130	LEU O	-20.88	-5.24	3.03	30.00
131	ALA N	-21.18	-4.82	4.64	30.00
131	ALA CA	-21.24	-6.27	4.85	30.00
131	ALA CB	-20.27	-6.70	5.94	30.00
131	ALA C	-22.65	-6.66	5.32	30.00
131	ALA O	-23.26	-5.92	6.11	30.00
132	THR N	-23.19	-7.71	4.76	30.00
132	THR CA	-24.55	-8.17	5.09	30.00
132	THR CB	-25.40	-8.32	3.81	30.00
132	THR OG1	-24.63	-8.99	2.82	30.00
132	THR CG2	-25.82	-6.95	3.28	30.00
132	THR C	-24.42	-9.54	5.77	30.00
132	THR O	-23.53	-10.32	5.43	30.00
133	ALA N	-25.27	-9.79	6.77	30.00
133	ALA CA	-25.27	-11.09	7.50	30.00
133	ALA CB	-25.97	-10.95	8.84	30.00

Fig. 7CC

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
133	ALA C	-25.98	-12.16	6.62	30.00
133	ALA O	-25.37	-13.21	6.33	30.00
144	THR N	-31.96	-6.77	10.16	30.00
144	THR CA	-30.60	-7.15	10.63	30.00
144	THR CB	-30.68	-8.37	11.59	30.00
144	THR OG1	-31.10	-9.53	10.86	30.00
144	THR CG2	-31.67	-8.11	12.71	30.00
144	THR C	-29.66	-7.54	9.45	30.00
144	THR O	-28.58	-8.11	9.64	30.00
145	LEU N	-30.11	-7.28	8.23	30.00
145	LEU CA	-29.33	-7.63	7.03	30.00
145	LEU CB	-30.17	-7.39	5.77	30.00
145	LEU CG	-29.51	-7.83	4.48	30.00
145	LEU CD1	-29.30	-9.30	4.48	30.00
145	LEU CD2	-30.34	-7.42	3.32	30.00
145	LEU C	-28.05	-6.49	6.64	30.00
145	LEU O	-26.92	-7.42	6.73	30.00
146	PHE N	-28.09	-5.22	7.07	30.00
146	PHE CA	-26.85	-4.45	7.20	30.00
146	PHE CB	-27.23	-2.99	7.26	30.00
146	PHE CG	-27.87	-2.56	5.95	30.00
146	PHE CD1	-28.29	-1.25	5.78	30.00
146	PHE CD2	-28.02	-3.47	4.94	30.00
146	PHE CE1	-28.85	-0.88	4.55	30.00
146	PHE CE2	-28.57	-3.10	3.73	30.00
146	PHE CZ	-28.99	-1.78	3.54	30.00
146	PHE C	-26.06	-4.91	8.43	30.00
146	PHE O	-26.50	-4.77	9.56	30.00
147	ALA N	-24.89	-5.47	8.17	30.00

Fig. 7DD

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
147	ALA CA	-23.95	-5.76	9.43	30.00
147	ALA CB	-23.08	-6.93	9.09	30.00
147	ALA C	-23.08	-4.55	9.81	30.00
147	ALA O	-23.10	-4.08	10.93	30.00
148	HIS N	-22.28	-4.06	8.86	30.00
148	HIS CA	-21.39	-2.88	9.07	30.00
148	HIS CB	-20.28	-3.23	10.04	30.00
148	HIS CG	-19.42	-4.37	9.58	30.00
148	HIS CD2	-19.55	-5.71	9.74	30.00
148	HIS ND1	-18.23	-4.18	8.90	30.00
148	HIS CE1	-17.67	-5.35	8.66	30.00
148	HIS NE2	-18.45	-6.30	9.16	30.00
148	HIS C	-20.78	-2.41	7.74	30.00
148	HIS O	-20.87	-3.07	6.68	30.00
149	VAL N	-20.13	-1.25	7.81	30.00
149	VAL CA	-19.46	-0.71	6.61	30.00
149	VAL CB	-20.03	0.65	6.15	30.00
149	VAL CG1	-21.50	0.69	6.42	30.00
149	VAL CG2	-19.31	1.80	6.78	30.00
149	VAL C	-17.98	-0.59	6.92	30.00
149	VAL O	-17.55	-0.23	8.02	30.00
150	ALA N	-17.18	-0.94	5.92	30.00
150	ALA CA	-15.75	-0.91	6.05	30.00
150	ALA CB	-15.18	-2.29	5.81	30.00
150	ALA C	-15.20	0.07	5.03	30.00
150	ALA O	-15.67	0.15	3.90	30.00
151	LEU N	-14.29	0.92	5.48	30.00
151	LEU CA	-13.61	1.88	4.61	30.00
151	LEU CB	-13.02	3.00	5.45	30.00

Fig. 7EE

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
151	LEU CG	-13.76	4.30	5.72	30.00
151	LEU CD1	-12.81	5.47	5.79	30.00
151	LEU CD2	-14.84	4.47	4.65	30.00
151	LEU C	-12.49	1.01	4.01	30.00
151	LEU O	-11.92	0.16	4.69	30.00
152	CYS N	-12.19	1.21	2.74	30.00
152	CYS CA	-11.12	0.42	2.10	30.00
152	CYS CB	-11.67	-0.96	1.79	30.00
152	CYS SG	-13.13	-0.89	0.76	30.00
152	CYS C	-10.63	1.13	0.86	30.00
152	CYS O	-11.10	2.19	0.50	30.00
153	ALA N	-9.66	0.54	0.19	30.00
153	ALA CA	-9.09	1.15	-1.03	30.00
153	ALA CB	-7.72	0.58	-1.30	30.00
153	ALA C	-9.96	0.94	-2.26	30.00
153	ALA O	-10.20	1.84	-3.04	30.00
154	ILE N	-10.41	-0.28	-2.44	30.00
154	ILE CA	-11.24	-0.63	-3.59	30.00
154	ILE CB	-10.34	-1.21	-4.74	30.00
154	ILE CG2	-11.16	-1.69	-5.88	30.00
154	ILE CG1	-9.35	-0.16	-5.27	30.00
154	ILE CD1	-10.00	1.00	-6.02	30.00
154	ILE C	-12.28	-1.66	-3.09	30.00
154	ILE O	-11.93	-2.72	-2.56	30.00
155	GLY N	-13.56	-1.30	-3.22	30.00
155	GLY CA	-14.66	-2.15	-2.80	30.00
155	GLY C	-15.01	-3.15	-3.87	30.00
155	GLY O	-14.49	-3.07	-4.99	30.00
156	ARG N	-15.93	-4.07	-3.57	30.00

Fig. 7FF

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
156	ARG CA	-16.32	-5.09	-4.56	30.00
156	ARG CB	-16.44	-6.44	-3.87	30.00
156	ARG CG	-15.72	-6.48	-2.54	30.00
156	ARG CD	-16.10	-7.68	-1.74	30.00
156	ARG NE	-15.93	-8.92	-2.48	30.00
156	ARG CZ	-15.62	-10.08	-1.91	30.00
156	ARG NH1	-15.48	-11.17	-2.65	30.00
156	ARG NH2	-15.44	-10.16	-0.59	30.00
156	ARG C	-17.57	-4.76	-5.40	30.00
156	ARG O	-17.83	-5.32	-6.46	30.00
157	ARG N	-18.38	-3.86	-4.89	30.00
157	ARG CA	-19.57	-3.45	-5.62	30.00
157	ARG CB	-20.72	-3.30	-4.65	30.00
157	ARG CG	-21.29	-4.64	-4.20	30.00
157	ARG CD	-22.70	-4.56	-3.58	30.00
157	ARG NE	-22.57	-4.44	-2.14	30.00
157	ARG CZ	-22.86	-5.36	-1.23	30.00
157	ARG NH1	-23.39	-6.54	-1.44	30.00
157	ARG NH2	-22.15	-5.29	-0.14	30.00
157	ARG C	-19.22	-2.14	-6.37	30.00
157	ARG O	-18.27	-1.44	-6.03	30.00
158	LEU N	-19.98	-1.85	-7.42	30.00
158	LEU CA	-19.76	-0.66	-8.25	30.00
158	LEU CB	-20.46	-0.84	-9.58	30.00
158	LEU CG	-19.65	-1.48	-10.69	30.00
158	LEU CD1	-18.52	-2.35	-10.15	30.00
158	LEU CD2	-20.57	-2.27	-11.56	30.00
158	LEU C	-20.19	0.64	-7.60	30.00
158	LEU O	-20.95	0.67	-6.64	30.00

Fig. 7GG

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
159 GLY N	-19.72	1.74	-8.18	30.00
159 GLY CA	-20.05	3.06	-7.69	30.00
159 GLY C	-19.85	3.34	-6.21	30.00
159 GLY O	-20.30	4.38	-5.72	30.00
160 THR N	-19.09	2.48	-5.53	30.00
160 THR CA	-18.86	2.67	-4.09	30.00
160 THR CB	-18.67	1.35	-3.38	30.00
160 THR OG1	-17.75	0.53	-4.12	30.00
160 THR CG2	-20.01	0.66	-3.21	30.00
160 THR C	-17.71	3.57	-3.73	30.00
160 THR O	-16.87	3.22	-2.93	30.00
161 ILE N	-17.68	4.76	-4.30	30.00
161 ILE CA	-16.62	5.69	-3.98	30.00
161 ILE CB	-16.13	6.37	-5.22	30.00
161 ILE CG2	-16.35	7.83	-5.13	30.00
161 ILE CG1	-14.65	6.06	-5.41	30.00
161 ILE CD1	-13.78	6.61	-4.37	30.00
161 ILE C	-17.25	6.69	-3.02	30.00
161 ILE O	-18.34	7.21	-3.30	30.00
162 VAL N	-16.59	6.92	-1.89	30.00
162 VAL CA	-17.11	7.86	-0.85	30.00
162 VAL CB	-17.01	7.27	0.57	30.00
162 VAL CG1	-17.75	5.96	0.66	30.00
162 VAL CG2	-15.56	7.10	0.96	30.00
162 VAL C	-16.45	9.24	-0.87	30.00
162 VAL O	-15.50	9.50	-1.58	30.00
163 THR N	-17.04	10.13	-0.07	30.00
163 THR CA	-16.61	11.54	0.10	30.00
163 THR CB	-17.72	12.50	-0.36	30.00

Fig. 7HH

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
163 THR OG1	-17.80	12.52	-1.79	30.00
163 THR CG2	-17.43	13.86	0.08	30.00
163 THR C	-16.43	11.76	1.61	30.00
163 THR O	-17.18	11.25	2.44	30.00
164 TYR N	-15.40	12.49	1.97	30.00
164 TYR CA	-15.10	12.87	3.35	30.00
164 TYR CB	-13.76	12.30	3.74	30.00
164 TYR CG	-13.75	10.79	3.68	30.00
164 TYR CD1	-14.55	10.17	2.76	30.00
164 TYR CE1	-14.53	8.79	2.70	30.00
164 TYR CD2	-12.94	10.09	4.54	30.00
164 TYR CE2	-12.92	8.72	4.50	30.00
164 TYR CZ	-13.72	8.07	3.58	30.00
164 TYR OH	-13.76	6.68	3.59	30.00
164 TYR C	-15.05	14.38	3.57	30.00
164 TYR O	-14.46	15.05	2.72	30.00
165 ASP N	-15.66	14.87	4.59	30.00
165 ASP CA	-15.57	16.32	4.83	30.00
165 ASP CB	-16.45	17.12	3.88	30.00
165 ASP CG	-15.75	18.39	3.40	30.00
165 ASP OD1	-15.57	19.33	4.19	30.00
165 ASP OD2	-15.37	18.45	2.22	30.00
165 ASP C	-15.91	16.62	6.27	30.00
165 ASP O	-16.35	15.74	7.00	30.00
166 THR N	-15.66	17.85	6.70	30.00
166 THR CA	-15.91	18.24	8.10	30.00
166 THR CB	-14.89	19.26	8.61	30.00
166 THR OG1	-14.86	20.39	7.71	30.00
166 THR CG2	-13.52	18.62	8.70	30.00

Fig. 7II

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
166 THR C	-17.32	18.80	8.34	30.00
166 THR O	-17.63	19.39	9.37	30.00
167 GLY N	-18.15	18.67	7.38	30.00
167 GLY CA	-19.54	19.03	7.44	30.00
167 GLY C	-20.42	18.10	6.67	30.00
167 GLY O	-19.91	17.60	5.64	30.00
168 LEU N	-21.53	17.72	7.17	30.00
168 LEU CA	-22.36	16.73	6.45	30.00
168 LEU CB	-23.59	16.37	7.29	30.00
168 LEU CG	-24.08	14.93	7.24	30.00
168 LEU CD1	-25.13	14.81	6.20	30.00
168 LEU CD2	-22.95	14.00	6.88	30.00
168 LEU C	-22.74	17.26	5.07	30.00
168 LEU O	-22.55	16.62	4.05	30.00
169 ASP N	-23.20	18.50	5.05	30.00
169 ASP CA	-23.62	19.19	3.81	30.00
169 ASP CB	-24.06	20.61	4.14	30.00
169 ASP CG	-25.51	20.70	4.54	30.00
169 ASP OD1	-26.07	21.82	4.51	30.00
169 ASP OD2	-26.11	19.67	4.88	30.00
169 ASP C	-22.51	19.20	2.75	30.00
169 ASP O	-22.75	19.02	1.56	30.00
170 ALA N	-21.28	19.38	3.22	30.00
170 ALA CA	-20.11	19.42	2.33	30.00
170 ALA CB	-18.95	20.04	3.03	30.00
170 ALA C	-19.72	18.04	1.83	30.00
170 ALA O	-19.12	17.89	0.77	30.00
171 ALA N	-20.05	17.03	2.62	30.00
171 ALA CA	-19.75	15.65	2.26	30.00

Fig. 7JJ

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
171 ALA CB	-19.78	14.79	3.50	30.00
171 ALA C	-20.77	15.15	1.22	30.00
171 ALA O	-20.46	14.35	0.34	30.00
172 ILE N	-22.02	15.61	1.32	30.00
172 ILE CA	-23.03	15.15	0.34	30.00
172 ILE CB	-24.45	14.96	0.98	30.00
172 ILE CG2	-25.14	13.81	0.32	30.00
172 ILE CG1	-24.39	14.65	2.47	30.00
172 ILE CD1	-25.76	14.42	3.09	30.00
172 ILE C	-23.12	15.98	-0.95	30.00
172 ILE O	-23.53	15.49	-2.00	30.00
173 ALA N	-22.66	17.23	-0.90	30.00
173 ALA CA	-22.70	18.14	-2.08	30.00
173 ALA CB	-22.11	19.49	-1.72	30.00
173 ALA C	-22.08	17.62	-3.39	30.00
173 ALA O	-22.53	17.97	-4.48	30.00
174 PRO N	-20.98	16.84	-3.32	30.00
174 PRO CD	-20.00	16.63	-2.25	30.00
174 PRO CA	-20.43	16.36	-4.59	30.00
174 PRO CB	-19.11	15.73	-4.20	30.00
174 PRO CG	-18.71	16.55	-3.05	30.00
174 PRO C	-21.32	15.32	-5.24	30.00
174 PRO O	-21.00	14.81	-6.30	30.00
175 PHE N	-22.38	14.92	-4.56	30.00
175 PHE CA	-23.30	13.94	-5.12	30.00
175 PHE CB	-23.81	13.03	-4.03	30.00
175 PHE CG	-22.78	12.08	-3.54	30.00
175 PHE CD1	-22.63	10.84	-4.16	30.00
175 PHE CD2	-21.93	12.44	-2.50	30.00

Fig. 7KK

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
175 PHE CE1	-21.64	9.97	-3.76	30.00
175 PHE CE2	-20.92	11.58	-2.08	30.00
175 PHE CZ	-20.78	10.33	-2.72	30.00
175 PHE C	-24.42	14.67	-5.84	30.00
175 PHE O	-25.35	15.19	-5.25	30.00
176 ARG N	-24.25	14.75	-7.16	30.00
176 ARG CA	-25.19	15.44	-8.04	30.00
176 ARG CB	-24.43	15.99	-9.22	30.00
176 ARG CG	-23.25	16.85	-8.83	30.00
176 ARG CD	-23.66	18.14	-8.20	30.00
176 ARG NE	-22.59	18.66	-7.37	30.00
176 ARG CZ	-21.69	19.57	-7.76	30.00
176 ARG NH1	-20.73	19.98	-6.94	30.00
176 ARG NH2	-21.78	20.08	-8.96	30.00
176 ARG C	-26.38	14.57	-8.50	30.00
176 ARG O	-27.43	15.07	-8.88	30.00
177 HIS N	-26.21	13.26	-8.53	30.00
177 HIS CA	-27.35	12.40	-8.96	30.00
177 HIS CB	-26.87	11.28	-9.87	30.00
177 HIS CG	-26.18	11.77	-11.11	30.00
177 HIS CD2	-25.28	11.16	-11.92	30.00
177 HIS ND1	-26.36	13.04	-11.61	30.00
177 HIS CE1	-25.60	13.20	-12.68	30.00
177 HIS NE2	-24.94	12.08	-12.89	30.00
177 HIS C	-28.02	11.84	-7.71	30.00
177 HIS O	-28.05	10.64	-7.47	30.00
178 LEU N	-28.54	12.75	-6.91	30.00
178 LEU CA	-29.20	12.37	-5.64	30.00
178 LEU CB	-28.33	12.82	-4.47	30.00

Fig. 7LL

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
178	LEU CG	-28.06	11.82	-3.34	30.00
178	LEU CD1	-27.32	10.62	-3.88	30.00
178	LEU CD2	-27.24	12.49	-2.27	30.00
178	LEU C	-30.61	12.96	-5.54	30.00
178	LEU O	-30.86	14.16	-5.72	30.00
179	SER N	-31.53	12.06	-5.32	30.00
179	SER CA	-32.92	12.54	-5.14	30.00
179	SER CB	-33.82	11.34	-4.79	30.00
179	SER OG	-35.07	11.91	-4.43	30.00
179	SER C	-33.03	13.57	-4.00	30.00
179	SER O	-32.28	13.48	-3.00	30.00
180	PRO N	-33.76	14.64	-4.22	30.00
180	PRO CD	-34.48	14.95	-5.47	30.00
180	PRO CA	-33.91	15.73	-3.26	30.00
180	PRO CB	-34.98	16.58	-3.91	30.00
180	PRO CG	-34.68	16.42	-5.36	30.00
180	PRO C	-34.37	15.21	-1.90	30.00
180	PRO O	-33.98	15.70	-0.85	30.00
181	ALA N	-35.23	14.21	-1.93	30.00
181	ALA CA	-35.75	13.59	-0.70	30.00
181	ALA CB	-36.78	12.54	-1.02	30.00
181	ALA C	-34.61	12.96	0.10	30.00
181	ALA O	-34.52	13.10	1.31	30.00
182	SER N	-33.68	12.50	-0.57	30.00
182	SER CA	-32.63	11.68	0.07	30.00
182	SER CB	-31.78	11.01	-1.02	30.00
182	SER OG	-30.49	10.84	-0.44	30.00
182	SER C	-31.69	12.51	0.96	30.00
182	SER O	-31.43	12.16	2.10	30.00

Fig. 7MM

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
183	ARG N	-31.50	13.75	0.23	30.00
183	ARG CA	-30.76	14.82	0.89	30.00
183	ARG CB	-30.57	15.98	-0.06	30.00
183	ARG CG	-29.34	15.87	-0.82	30.00
183	ARG CD	-29.53	16.56	-2.10	30.00
183	ARG NE	-29.90	17.94	-1.83	30.00
183	ARG CZ	-29.40	18.98	-2.48	30.00
183	ARG NH1	-29.80	20.21	-2.16	30.00
183	ARG NH2	-28.50	18.80	-3.44	30.00
183	ARG C	-31.48	15.29	2.14	30.00
183	ARG O	-30.93	15.32	3.23	30.00
184	GLU N	-32.74	15.64	1.98	30.00
184	GLU CA	-33.53	16.13	3.13	30.00
184	GLU CB	-34.86	16.70	2.63	30.00
184	GLU CG	-35.68	17.41	3.73	30.00
184	GLU CD	-35.24	18.89	3.97	30.00
184	GLU OE1	-34.03	19.13	4.23	30.00
184	GLU OE2	-36.10	19.80	3.90	30.00
184	GLU C	-33.73	15.09	4.27	30.00
184	GLU O	-33.87	15.41	5.45	30.00
185	GLY N	-33.67	13.83	3.89	30.00
185	GLY CA	-33.87	12.78	4.87	30.00
185	GLY C	-32.58	12.41	5.57	30.00
185	GLY O	-32.57	12.14	6.76	30.00
186	ALA N	-31.48	12.44	4.83	30.00
186	ALA CA	-30.18	12.04	5.37	30.00
186	ALA CB	-29.19	11.86	4.31	30.00
186	ALA C	-29.66	13.12	6.32	30.00
186	ALA O	-28.84	12.86	7.21	30.00

Fig. 7NN

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
187 ARG N	-30.12	14.34	6.12	30.00
187 ARG CA	-29.73	15.48	6.98	30.00
187 ARG CB	-30.04	16.80	6.29	30.00
187 ARG CG	-29.13	17.18	5.17	30.00
187 ARG CD	-29.47	18.59	4.71	30.00
187 ARG NE	-28.59	19.06	3.64	30.00
187 ARG CZ	-29.01	19.37	2.41	30.00
187 ARG NH1	-28.13	19.78	1.51	30.00
187 ARG NH2	-30.29	19.26	2.08	30.00
187 ARG C	-30.50	15.42	8.31	30.00
187 ARG O	-30.00	15.74	9.39	30.00
188 ARG N	-31.78	15.05	8.20	30.00
188 ARG CA	-32.69	14.95	9.35	30.00
188 ARG CB	-34.12	14.76	8.85	30.00
188 ARG CG	-35.20	15.12	9.87	30.00
188 ARG CD	-36.22	14.00	10.04	30.00
188 ARG NE	-36.68	13.52	8.74	30.00
188 ARG CZ	-36.76	12.23	8.39	30.00
188 ARG NH1	-37.19	11.91	7.17	30.00
188 ARG NH2	-36.41	11.28	9.25	30.00
188 ARG C	-32.26	13.80	10.28	30.00
188 ARG O	-32.02	13.98	11.45	30.00
189 LEU N	-32.09	12.61	9.73	30.00
189 LEU CA	-31.73	11.47	10.54	30.00
189 LEU CB	-31.74	10.19	9.64	30.00
189 LEU CG	-32.07	8.79	10.13	30.00
189 LEU CD1	-30.97	7.78	9.86	30.00
189 LEU CD2	-32.41	8.89	11.58	30.00
189 LEU C	-30.34	11.71	11.11	30.00

Fig. 700

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
189	LEU O	-30.13	11.50	12.31	30.00
190	ALA N	-29.39	12.11	10.30	30.00
190	ALA CA	-27.98	12.32	10.76	30.00
190	ALA CB	-27.12	12.77	9.62	30.00
190	ALA C	-27.83	13.26	11.98	30.00
190	ALA O	-26.99	13.04	12.86	30.00
191	ALA N	-28.66	14.29	12.03	30.00
191	ALA CA	-28.63	15.27	13.16	30.00
191	ALA CB	-29.49	16.43	12.84	30.00
191	ALA C	-29.10	14.62	14.49	30.00
191	ALA O	-28.57	14.85	15.58	30.00
192	GLU N	-30.17	13.84	14.38	30.00
192	GLU CA	-30.71	13.15	15.54	30.00
192	GLU CB	-32.03	12.48	15.19	30.00
192	GLU CG	-33.14	13.45	14.79	30.00
192	GLU CD	-34.48	12.74	14.47	30.00
192	GLU OE1	-34.56	11.49	14.60	30.00
192	GLU OE2	-35.44	13.46	14.09	30.00
192	GLU C	-29.69	12.13	15.99	30.00
192	GLU O	-29.21	12.16	17.11	30.00
193	ALA N	-29.32	11.26	15.07	30.00
193	ALA CA	-28.33	10.18	15.33	30.00
193	ALA CB	-27.93	9.51	14.05	30.00
193	ALA C	-27.09	10.73	16.02	30.00
193	ALA O	-26.55	10.13	16.95	30.00
194	GLU N	-26.65	11.89	15.56	30.00
194	GLU CA	-25.48	12.52	16.17	30.00
194	GLU CB	-25.10	13.77	15.43	30.00
194	GLU CG	-24.26	13.53	14.25	30.00

Fig. 7PP

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
194 GLU CD	-23.81	14.81	13.68	30.00
194 GLU OE1	-24.44	15.29	12.71	30.00
194 GLU OE2	-22.83	15.37	14.24	30.00
194 GLU C	-25.67	12.84	17.63	30.00
194 GLU O	-24.75	12.75	18.43	30.00
195 LEU N	-26.87	13.29	17.97	30.00
195 LEU CA	-27.20	13.63	19.36	30.00
195 LEU CB	-28.66	14.02	19.45	30.00
195 LEU CG	-28.93	15.39	18.85	30.00
195 LEU CD1	-30.38	15.76	19.00	30.00
195 LEU CD2	-28.05	16.38	19.59	30.00
195 LEU C	-26.88	12.51	20.33	30.00
195 LEU O	-26.43	12.73	21.45	30.00
196 ALA N	-27.16	11.28	19.91	30.00
196 ALA CA	-26.88	10.11	20.74	30.00
196 ALA CB	-27.44	8.86	20.10	30.00
196 ALA C	-25.35	9.98	20.93	30.00
196 ALA O	-24.78	10.36	21.94	30.00
197 LEU N	-24.68	9.51	19.88	30.00
197 LEU CA	-23.20	9.33	19.96	30.00
197 LEU CB	-22.69	8.39	18.84	30.00
197 LEU CG	-22.63	8.69	17.34	30.00
197 LEU CD1	-23.69	9.67	16.99	30.00
197 LEU CD2	-21.28	9.23	16.93	30.00
197 LEU C	-22.47	10.67	19.98	30.00
197 LEU O	-21.34	10.81	19.51	30.00
198 SER N	-23.19	11.66	20.51	30.00
198 SER CA	-22.53	12.98	20.64	30.00
198 SER CB	-23.57	14.03	21.05	30.00

Fig. 7QQ

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
198	SER OG	-22.90	14.87	21.98	30.00
198	SER C	-21.41	12.96	21.68	30.00
198	SER O	-21.66	12.48	22.78	30.00
199	GLY N	-20.26	13.22	21.20	30.00
199	GLY CA	-19.11	13.17	22.08	30.00
199	GLY C	-18.31	11.88	21.92	30.00
199	GLY O	-17.14	11.84	22.29	30.00
200	ARG N	-18.92	10.83	21.39	30.00
200	ARG CA	-18.18	9.60	21.25	30.00
200	ARG CB	-19.08	8.47	20.82	30.00
200	ARG CG	-18.32	7.22	20.59	30.00
200	ARG CD	-19.19	6.00	20.73	30.00
200	ARG NE	-18.40	4.87	21.18	30.00
200	ARG CZ	-18.81	3.61	21.18	30.00
200	ARG NH1	-18.01	2.64	21.60	30.00
200	ARG NH2	-20.04	3.31	20.76	30.00
200	ARG C	-17.02	9.74	20.27	30.00
200	ARG O	-17.09	10.38	19.22	30.00
201	THR N	-15.90	9.17	20.71	30.00
201	THR CA	-14.65	9.12	19.97	30.00
201	THR CB	-13.56	9.86	20.72	30.00
201	THR OG1	-13.94	11.22	20.82	30.00
201	THR CG2	-12.20	9.77	19.96	30.00
201	THR C	-14.31	7.66	20.01	30.00
201	THR O	-14.65	6.95	20.96	30.00
202	TRP N	-13.67	7.18	18.95	30.00
202	TRP CA	-13.27	5.79	18.91	30.00
202	TRP CB	-13.67	5.21	17.56	30.00
202	TRP CG	-15.19	5.16	17.37	30.00

Fig. 7RR

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
202	TRP CD2	-16.07	6.26	17.09	30.00
202	TRP CE2	-17.39	5.75	17.05	30.00
202	TRP CE3	-15.88	7.62	16.87	30.00
202	TRP CD1	-15.99	4.04	17.46	30.00
202	TRP NE1	-17.31	4.40	17.29	30.00
202	TRP CZ2	-18.49	6.55	16.81	30.00
202	TRP CZ3	-16.99	8.41	16.62	30.00
202	TRP CH2	-18.27	7.88	16.60	30.00
202	TRP C	-11.77	5.81	19.15	30.00
202	TRP O	-11.11	6.82	19.02	30.00
203	ALA N	-11.22	4.70	19.61	30.00
203	ALA CA	-9.76	4.62	19.85	30.00
203	ALA CB	-9.43	5.17	21.19	30.00
203	ALA C	-9.36	3.16	19.76	30.00
203	ALA O	-9.09	2.48	20.75	30.00
204	PRO N	-9.30	2.64	18.53	30.00
204	PRO CD	-9.63	3.34	17.27	30.00
204	PRO CA	-8.95	1.24	18.26	30.00
204	PRO CB	-9.25	1.10	16.76	30.00
204	PRO CG	-9.02	2.46	16.24	30.00
204	PRO C	-7.53	0.77	18.65	30.00
204	PRO O	-7.29	-0.42	18.88	30.00
205	GLY N	-6.61	1.72	18.77	30.00
205	GLY CA	-5.23	1.42	19.12	30.00
205	GLY C	-4.33	1.80	17.96	30.00
205	GLY O	-4.45	1.21	16.90	30.00
206	VAL N	-3.39	2.73	18.16	30.00
206	VAL CA	-2.53	3.18	17.05	30.00
206	VAL CB	-1.56	4.34	17.42	30.00

Fig. 7SS

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
206 VAL CG1	-0.15	3.83	17.65	30.00
206 VAL CG2	-1.56	5.38	16.40	30.00
206 VAL C	-1.81	2.04	16.35	30.00
206 VAL O	-1.73	2.00	15.13	30.00
207 GLU N	-1.34	1.06	17.11	30.00
207 GLU CA	-0.66	-0.06	16.44	30.00
207 GLU CB	0.10	-0.94	17.42	30.00
207 GLU CG	1.38	-0.31	17.97	30.00
207 GLU CD	2.12	0.58	16.97	30.00
207 GLU OE1	2.24	0.24	15.77	30.00
207 GLU OE2	2.61	1.64	17.40	30.00
207 GLU C	-1.64	-0.89	15.61	30.00
207 GLU O	-1.33	-1.33	14.51	30.00
208 ALA N	-2.84	-1.09	16.16	30.00
208 ALA CA	-3.90	-1.84	15.47	30.00
208 ALA CB	-5.16	-1.86	16.29	30.00
208 ALA C	-4.15	-1.08	14.16	30.00
208 ALA O	-4.16	-1.64	13.07	30.00
209 LEU N	-4.28	0.23	14.31	30.00
209 LEU CA	-4.52	1.10	13.16	30.00
209 LEU CB	-4.71	2.52	13.63	30.00
209 LEU CG	-6.18	2.79	13.90	30.00
209 LEU CD1	-6.38	4.15	14.51	30.00
209 LEU CD2	-6.91	2.64	12.60	30.00
209 LEU C	-3.39	1.02	12.16	30.00
209 LEU O	-3.57	0.88	10.96	30.00
210 THR N	-2.18	1.07	12.70	30.00
210 THR CA	-0.99	1.05	11.85	30.00
210 THR CB	0.27	1.27	12.72	30.00

Fig. 7TT

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
210	THR OG1	0.25	2.60	13.26	30.00
210	THR CG2	1.52	1.13	11.90	30.00
210	THR C	-0.92	-0.26	11.05	30.00
210	THR O	-0.74	-0.27	9.85	30.00
211	HIS N	-1.13	-1.37	11.74	30.00
211	HIS CA	-1.05	-2.69	11.08	30.00
211	HIS CB	-1.05	-3.83	12.13	30.00
211	HIS CG	-0.99	-5.21	11.53	30.00
211	HIS CD2	-1.96	-5.99	10.99	30.00
211	HIS ND1	0.17	-5.95	11.46	30.00
211	HIS CE1	-0.08	-7.12	10.91	30.00
211	HIS NE2	-1.36	-7.17	10.62	30.00
211	HIS C	-2.16	-2.85	10.05	30.00
211	HIS O	-1.93	-3.30	8.92	30.00
212	THR N	-3.36	-2.40	10.40	30.00
212	THR CA	-4.55	-2.51	9.50	30.00
212	THR CB	-5.87	-2.09	10.23	30.00
212	THR OG1	-6.17	-3.05	11.24	30.00
212	THR CG2	-7.04	-2.06	9.31	30.00
212	THR C	-4.36	-1.75	8.15	30.00
212	THR O	-4.72	-2.21	7.07	30.00
213	LEU N	-3.77	-0.56	8.24	30.00
213	LEU CA	-3.51	0.24	7.06	30.00
213	LEU CB	-3.27	1.65	7.49	30.00
213	LEU CG	-4.51	2.33	8.09	30.00
213	LEU CD1	-4.11	3.73	8.56	30.00
213	LEU CD2	-5.62	2.44	7.07	30.00
213	LEU C	-2.34	-0.33	6.20	30.00
213	LEU O	-2.33	-0.25	4.97	30.00

Fig. 7UU

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
214 LEU N	-1.38	-0.97	6.84	30.00
214 LEU CA	-0.26	-1.57	6.10	30.00
214 LEU CB	0.75	-2.18	7.05	30.00
214 LEU CG	2.20	-2.33	6.60	30.00
214 LEU CD1	2.74	-3.56	7.23	30.00
214 LEU CD2	2.33	-2.42	5.09	30.00
214 LEU C	-0.92	-2.67	5.29	30.00
214 LEU O	-0.70	-2.85	4.11	30.00
215 SER N	-1.77	-3.43	5.97	30.00
215 SER CA	-2.55	-4.55	5.34	30.00
215 SER CB	-3.46	-5.17	6.40	30.00
215 SER OG	-3.71	-6.53	6.16	30.00
215 SER C	-3.38	-4.06	4.11	30.00
215 SER O	-3.49	-4.71	3.07	30.00
216 THR N	-4.00	-2.90	4.25	30.00
216 THR CA	-4.78	-2.31	3.14	30.00
216 THR CB	-5.38	-0.94	3.56	30.00
216 THR OG1	-6.38	-1.16	4.56	30.00
216 THR CG2	-6.01	-0.21	2.39	30.00
216 THR C	-3.84	-2.11	1.90	30.00
216 THR O	-4.20	-2.34	0.75	30.00
217 ALA N	-2.60	-1.72	2.16	30.00
217 ALA CA	-1.62	-1.50	1.09	30.00
217 ALA CB	-0.45	-0.67	1.61	30.00
217 ALA C	-1.10	-2.83	0.55	30.00
217 ALA O	-1.15	-3.11	-0.64	30.00
218 VAL N	-0.60	-3.68	1.44	30.00
218 VAL CA	-0.02	-4.95	1.02	30.00
218 VAL CB	0.55	-5.74	2.21	30.00

Fig. 7VV

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
218	VAL CG1	0.83	-7.16	1.79	30.00
218	VAL CG2	1.86	-5.09	2.67	30.00
218	VAL C	-0.99	-5.80	0.21	30.00
218	VAL O	-0.66	-6.36	-0.82	30.00
219	ASN N	-2.23	-5.81	0.63	30.00
219	ASN CA	-3.25	-6.61	-0.07	30.00
219	ASN CB	-4.43	-6.87	0.84	30.00
219	ASN CG	-4.14	-7.91	1.84	30.00
219	ASN OD1	-3.77	-9.04	1.50	30.00
219	ASN ND2	-4.28	-7.55	3.10	30.00
219	ASN C	-3.76	-6.04	-1.41	30.00
219	ASN O	-4.48	-6.68	-2.16	30.00
220	ASN N	-3.41	-4.79	-1.68	30.00
220	ASN CA	-3.85	-4.16	-2.92	30.00
220	ASN CB	-4.66	-2.90	-2.62	30.00
220	ASN CG	-6.05	-3.21	-2.10	30.00
220	ASN OD1	-7.00	-3.40	-2.88	30.00
220	ASN ND2	-6.20	-3.25	-0.77	30.00
220	ASN C	-2.67	-3.80	-3.82	30.00
220	ASN O	-2.83	-3.08	-4.81	30.00
221	MET N	-1.49	-4.31	-3.48	30.00
221	MET CA	-0.25	-4.00	-4.26	30.00
221	MET CB	0.98	-4.51	-3.53	30.00
221	MET CG	1.05	-5.99	-3.42	30.00
221	MET SD	2.55	-6.42	-2.70	30.00
221	MET CE	2.18	-7.97	-1.97	30.00
221	MET C	-0.30	-4.55	-5.68	30.00
221	MET O	0.13	-3.93	-6.63	30.00
222	MET N	-0.90	-5.72	-5.81	30.00

Fig. 7WW

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
222 MET CA	-1.01	-6.40	-7.12	30.00
222 MET CB	-1.21	-7.89	-6.86	30.00
222 MET CG	-0.08	-8.49	-6.04	30.00
222 MET SD	1.41	-8.81	-7.00	30.00
222 MET CE	1.82	-7.35	-7.59	30.00
222 MET C	-2.08	-5.84	-8.08	30.00
222 MET O	-2.34	-6.33	-9.16	30.00
223 LEU N	-2.69	-4.75	-7.67	30.00
223 LEU CA	-3.72	-4.14	-8.48	30.00
223 LEU CB	-4.63	-3.28	-7.58	30.00
223 LEU CG	-6.03	-3.76	-7.16	30.00
223 LEU CD1	-6.98	-3.60	-8.31	30.00
223 LEU CD2	-5.99	-5.23	-6.75	30.00
223 LEU C	-3.03	-3.30	-9.55	30.00
223 LEU O	-2.15	-2.47	-9.29	30.00
224 ARG N	-3.37	-3.60	-10.79	30.00
224 ARG CA	-2.84	-2.83	-11.92	30.00
224 ARG CB	-3.00	-3.64	-13.20	30.00
224 ARG CG	-2.15	-4.88	-13.22	30.00
224 ARG CD	-0.72	-4.52	-12.84	30.00
224 ARG NE	0.30	-5.34	-13.48	30.00
224 ARG CZ	0.43	-6.66	-13.35	30.00
224 ARG NH1	1.42	-7.28	-13.99	30.00
224 ARG NH2	-0.42	-7.37	-12.60	30.00
224 ARG C	-3.62	-1.51	-11.98	30.00
224 ARG O	-4.83	-1.48	-12.19	30.00
225 ASP N	-2.90	-0.43	-11.70	30.00
225 ASP CA	-3.50	0.95	-11.69	30.00
225 ASP CB	-3.65	1.46	-13.12	30.00

Fig. 7XX

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
225 ASP CG	-3.92	2.96	-13.18	30.00
225 ASP OD1	-3.84	3.62	-12.13	30.00
225 ASP OD2	-4.24	3.50	-14.26	30.00
225 ASP C	-4.87	1.05	-10.98	30.00
225 ASP O	-5.90	1.08	-11.60	30.00
226 ARG N	-4.91	1.22	-9.67	30.00
226 ARG CA	-6.23	1.29	-9.02	30.00
226 ARG CB	-6.03	1.13	-7.52	30.00
226 ARG CG	-4.69	1.68	-7.09	30.00
226 ARG CD	-4.23	1.22	-5.72	30.00
226 ARG NE	-4.53	2.27	-4.75	30.00
226 ARG CZ	-5.55	2.22	-3.91	30.00
226 ARG NH1	-5.77	3.23	-3.09	30.00
226 ARG NH2	-6.32	1.13	-3.86	30.00
226 ARG C	-7.01	2.59	-9.32	30.00
226 ARG O	-8.23	2.67	-9.14	30.00
227 TRP N	-6.28	3.63	-9.73	30.00
227 TRP CA	-6.90	4.95	-10.02	30.00
227 TRP CB	-5.81	6.01	-10.17	30.00
227 TRP CG	-5.62	6.85	-8.96	30.00
227 TRP CD2	-5.41	6.41	-7.61	30.00
227 TRP CE2	-5.23	7.56	-6.80	30.00
227 TRP CE3	-5.36	5.14	-7.00	30.00
227 TRP CD1	-5.57	8.22	-8.91	30.00
227 TRP NE1	-5.33	8.65	-7.63	30.00
227 TRP CZ2	-5.00	7.49	-5.42	30.00
227 TRP CZ3	-5.13	5.08	-5.61	30.00
227 TRP CH2	-4.95	6.25	-4.85	30.00
227 TRP C	-7.88	4.99	-11.21	30.00

Fig. 7YY

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
227 TRP O	-8.68	5.92	-11.38	30.00
228 SER N	-7.78	3.98	-12.06	30.00
228 SER CA	-8.67	3.87	-13.20	30.00
228 SER CB	-8.18	2.78	-14.13	30.00
228 SER OG	-7.15	3.28	-14.94	30.00
228 SER C	-10.03	3.51	-12.64	30.00
228 SER O	-11.05	4.14	-12.93	30.00
229 LEU N	-10.02	2.48	-11.80	30.00
229 LEU CA	-11.25	2.02	-11.16	30.00
229 LEU CB	-10.99	0.85	-10.23	30.00
229 LEU CG	-10.21	-0.32	-10.79	30.00
229 LEU CD1	-10.40	-1.52	-9.85	30.00
229 LEU CD2	-10.70	-0.65	-12.19	30.00
229 LEU C	-11.86	3.17	-10.37	30.00
229 LEU O	-13.04	3.46	-10.45	30.00
230 VAL N	-11.01	3.85	-9.61	30.00
230 VAL CA	-11.49	4.96	-8.78	30.00
230 VAL CB	-10.33	5.57	-7.93	30.00
230 VAL CG1	-10.80	6.79	-7.14	30.00
230 VAL CG2	-9.79	4.52	-6.97	30.00
230 VAL C	-12.21	6.00	-9.67	30.00
230 VAL O	-13.36	6.42	-9.45	30.00
231 ALA N	-11.56	6.31	-10.77	30.00
231 ALA CA	-12.10	7.30	-11.70	30.00
231 ALA CB	-11.11	7.53	-12.80	30.00
231 ALA C	-13.43	6.82	-12.27	30.00
231 ALA O	-14.45	7.50	-12.30	30.00
232 GLU N	-13.42	5.55	-12.64	30.00
232 GLU CA	-14.58	4.95	-13.22	30.00

Fig. 7ZZ

<u>Residue Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
232 GLU CB	-14.20	3.57	-13.73	30.00
232 GLU CG	-15.10	3.11	-14.82	30.00
232 GLU CD	-14.76	1.72	-15.32	30.00
232 GLU OE1	-15.38	0.74	-14.83	30.00
232 GLU OE2	-13.86	1.59	-16.18	30.00
232 GLU C	-15.92	4.63	-12.26	30.00
232 GLU O	-16.89	5.30	-12.58	30.00
233 ARG N	-15.48	4.47	-11.02	30.00
233 ARG CA	-16.55	4.32	-9.97	30.00
233 ARG CB	-16.11	3.29	-8.95	30.00
233 ARG CG	-15.92	1.94	-9.62	30.00
233 ARG CD	-14.70	1.20	-9.19	30.00
233 ARG NE	-14.85	-0.22	-9.46	30.00
233 ARG CZ	-14.72	-1.19	-8.56	30.00
233 ARG NH1	-14.89	-2.46	-8.93	30.00
233 ARG NH2	-14.39	-0.91	-7.31	30.00
233 ARG C	-16.98	5.65	-9.36	30.00
233 ARG O	-18.05	5.78	-8.76	30.00
234 ARG N	-16.76	6.50	-9.75	30.00
234 ARG CA	-16.48	8.02	-9.11	30.00
234 ARG CB	-15.25	8.92	-9.19	30.00
234 ARG CG	-15.60	10.38	-8.97	30.00
234 ARG CD	-14.57	11.42	-9.43	30.00
234 ARG NE	-15.13	12.76	-9.21	30.00
234 ARG CZ	-14.48	13.83	-8.74	30.00
234 ARG NH1	-13.20	13.78	-8.43	30.00
234 ARG NH2	-15.14	14.96	-8.51	30.00
234 ARG C	-17.57	8.52	-10.08	30.00
234 ARG O	-18.51	9.23	-9.70	30.00

Fig. 7AAA

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
235 ARG N	-17.40	8.19	-11.37	30.00
235 ARG CA	-18.36	8.59	-12.46	30.00
235 ARG CB	-17.76	8.29	-13.82	30.00
235 ARG CG	-16.50	9.12	-14.10	30.00
235 ARG CD	-16.08	9.07	-15.56	30.00
235 ARG NE	-15.88	7.69	-16.00	30.00
235 ARG CZ	-14.68	7.14	-16.20	30.00
235 ARG NH1	-14.60	5.87	-16.60	30.00
235 ARG NH2	-13.57	7.85	-16.01	30.00
235 ARG C	-19.70	7.91	-12.32	30.00
235 ARG O	-20.75	8.52	-12.44	30.00
236 GLN N	-19.66	6.61	-12.05	30.00
236 GLN CA	-20.89	5.80	-11.81	30.00
236 GLN CB	-20.53	4.34	-11.51	30.00
236 GLN CG	-19.31	3.77	-12.26	30.00
236 GLN CD	-19.28	2.25	-12.26	30.00
236 GLN OE1	-18.36	1.64	-12.82	30.00
236 GLN NE2	-20.29	1.62	-11.65	30.00
236 GLN C	-21.73	6.36	-10.64	30.00
236 GLN O	-22.94	6.21	-10.61	30.00
237 ALA N	-21.04	6.92	-9.64	30.00
237 ALA CA	-21.70	7.50	-8.40	30.00
237 ALA CB	-20.70	7.53	-7.24	30.00
237 ALA C	-22.30	8.89	-8.61	30.00
237 ALA O	-23.09	9.39	-7.82	30.00
238 GLY N	-21.89	9.54	-9.70	30.00
238 GLY CA	-22.39	10.86	-10.00	30.00
238 GLY C	-21.68	11.89	-9.14	30.00
238 GLY O	-22.25	12.93	-8.84	30.00

Fig. 7BBB

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
239	ILE N	-20.44	11.58	-8.74	30.00
239	ILE CA	-19.61	12.49	-7.87	30.00
239	ILE CB	-18.48	11.72	-7.08	30.00
239	ILE CG2	-17.66	12.66	-6.26	30.00
239	ILE CG1	-19.07	10.71	-6.11	30.00
239	ILE CD1	-18.02	9.87	-5.50	30.00
239	ILE C	-18.94	13.43	-8.82	30.00
239	ILE O	-18.33	13.03	-9.83	30.00
240	ALA N	-19.01	14.71	-8.48	30.00
240	ALA CA	-18.40	15.73	-9.31	30.00
240	ALA CB	-19.35	16.10	-10.46	30.00
240	ALA C	-18.10	16.97	-8.50	30.00
240	ALA O	-18.78	17.31	-7.53	30.00
241	GLY N	-17.05	17.66	-8.91	30.00
241	GLY CA	-16.70	18.87	-8.21	30.00
241	GLY C	-15.25	18.93	-7.84	30.00
241	GLY O	-14.41	18.20	-8.34	30.00
242	HIS N	-14.95	19.87	-6.97	30.00
242	HIS CA	-13.60	20.10	-6.50	30.00
242	HIS CB	-13.47	21.56	-6.11	30.00
242	HIS CG	-12.12	22.14	-6.36	30.00
242	HIS CD2	-11.42	23.09	-5.70	30.00
242	HIS ND1	-11.33	21.73	-7.41	30.00
242	HIS CE1	-10.19	22.41	-7.38	30.00
242	HIS NE2	-10.22	23.23	-6.36	30.00
242	HIS C	-13.39	19.17	-5.31	30.00
242	HIS O	-13.38	19.57	-4.15	30.00
243	THR N	-13.30	17.88	-5.61	30.00
243	THR CA	-13.11	16.89	-4.55	30.00

Fig. 7CCC

<u>Residue</u>	<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
243	THR CB	-13.77	15.55	-4.95	30.00
243	THR OG1	-15.02	15.80	-5.62	30.00
243	THR CG2	-14.03	14.69	-3.69	30.00
243	THR C	-11.60	16.72	-4.22	30.00
243	THR O	-10.73	17.15	-4.97	30.00
244	TYR N	-11.30	16.18	-3.03	30.00
244	TYR CA	-9.88	15.93	-2.62	30.00
244	TYR CB	-9.73	15.68	-1.13	30.00
244	TYR CG	-10.06	16.83	-0.23	30.00
244	TYR CD1	-9.57	16.89	1.07	30.00
244	TYR CE1	-9.92	17.93	1.90	30.00
244	TYR CD2	-10.90	17.83	-0.68	30.00
244	TYR CE2	-11.26	18.87	0.14	30.00
244	TYR CZ	-10.77	18.90	1.43	30.00
244	TYR OH	-11.15	19.93	2.24	30.00
244	TYR C	-9.40	14.70	-3.34	30.00
244	TYR O	-8.22	14.42	-3.44	30.00
245	LEU N	-10.37	13.87	-3.73	30.00
245	LEU CA	-10.09	12.62	-4.45	30.00
245	LEU CB	-11.38	11.90	-4.78	30.00
245	LEU CG	-11.18	10.60	-5.55	30.00
245	LEU CD1	-10.17	9.70	-4.85	30.00
245	LEU CD2	-12.49	9.92	-5.70	30.00
245	LEU C	-9.35	13.03	-5.70	30.00
245	LEU O	-9.87	13.74	-6.55	30.00
246	GLN N	-8.14	12.53	-5.84	30.00
246	GLN CA	-7.25	12.88	-6.97	30.00
246	GLN CB	-5.80	12.76	-6.48	30.00
246	GLN CG	-5.04	14.07	-6.37	30.00

Fig. 7DDD

<u>Residue</u> <u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>B</u>
246 GLN CD	-5.89	15.30	-6.68	30.00
246 GLN OE1	-5.60	16.42	-6.26	30.00
246 GLN NE2	-6.96	15.09	-7.42	30.00
246 GLN C	-7.50	12.06	-8.25	30.00
246 GLN O	-6.59	11.75	-9.03	30.00
247 ALA N	-8.76	11.76	-8.50	30.00
247 ALA CA	-9.15	10.95	-9.65	30.00
247 ALA CB	-9.05	9.48	-9.29	30.00
247 ALA C	-10.58	11.28	-10.04	30.00
247 ALA O	-11.04	10.81	-11.10	30.00
247 ALA OT	-11.22	12.01	-9.27	30.00

Fig. 8A

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 N	128 C	1.311	129 N	128 O	2.215
129 N	128 CA	2.359	129 N	128 CB	2.891
129 N	150 O	2.902	129 N	130 N	3.249
129 N	128 N	3.556	129 N	128 CG1	3.899
129 N	128 CG2	3.930	129 N	150 C	4.033
129 N	150 N	4.141	129 N	300 OH2	4.223
129 N	301 OH2	4.344	129 N	127 C	4.448
129 N	130 CA	4.510	129 N	152 SG	4.570
129 N	127 O	4.573	129 N	150 CA	4.622
129 N	150 CB	4.975	129 N	149 C	5.116
129 N	149 CB	5.120	129 N	151 N	5.126
129 N	149 CA	5.155	129 N	130 CB	5.405
129 N	151 CA	5.411	129 N	27 CD1	5.447
129 N	130 C	5.492	129 N	155 CA	5.693
129 N	61 CE1	5.719	129 N	152 N	5.729
129 N	127 CA	5.740	129 N	151 C	5.742
129 N	127 CB	5.749	129 N	149 CG2	5.756
129 N	61 NE2	5.828	129 N	130 O	5.858
129 N	152 CB	5.908	129 N	27 O	6.138
129 N	149 CG1	6.179	129 N	149 O	6.208
129 N	131 N	6.263	129 N	151 O	6.377
129 N	148 O	6.406	129 N	27 CA	6.428
129 N	151 CD1	6.441	129 N	27 CG	6.469
129 N	155 N	6.481	129 N	152 CA	6.521
129 N	149 N	6.555	129 N	156 N	6.645
129 N	61 ND1	6.681	129 N	27 C	6.762
129 N	155 C	6.764	129 N	151 CB	6.810
129 N	130 CG	6.847	129 N	61 CD2	6.875
129 N	27 CB	6.882	129 N	157 NH2	6.887
129 N	131 OG	6.941	129 N	148 C	6.997
129 N	127 N	7.007	129 N	127 OG	7.076
129 N	152 O	7.143	129 N	130 CD1	7.157
129 N	152 C	7.198	129 N	151 CG	7.288
129 N	154 C	7.303	129 N	61 CG	7.352
129 N	154 O	7.459	129 N	27 N	7.468
129 N	131 CA	7.475	129 N	157 NE	7.478
129 N	157 N	7.533	129 N	157 CB	7.706
129 N	157 CZ	7.778	129 N	130 CD2	7.798
129 N	27 CD2	7.821	129 N	131 CB	7.825
129 N	155 O	7.887	129 N	157 O	7.932
129 N	156 CA	7.938	129 N	148 ND1	8.000
129 N	61 N	8.102	129 N	157 CG	8.181
129 N	60 N	8.218	129 N	157 CA	8.235
129 N	156 CB	8.281	129 N	154 CA	8.326
129 N	154 N	8.327	129 N	60 CA	8.331
129 N	156 C	8.365	129 N	148 CE1	8.374

Fig. 8B

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 N	156 CG	8.442	129 N	157 CD	8.471
129 N	157 C	8.503	129 N	148 CA	8.529
129 N	61 CB	8.591	129 N	151 CD2	8.642
129 N	131 C	8.679	129 N	61 CA	8.718
129 N	60 C	8.808	129 N	60 OD1	8.832
129 N	148 CG	8.855	129 N	131 O	8.939
129 N	157 NH1	8.984	129 N	148 CB	9.068
129 N	148 N	9.181	129 N	148 NE2	9.376
129 N	60 CB	9.492	129 N	156 O	9.565
129 N	132 N	9.587	129 N	60 CG	9.644
129 N	148 CD2	9.666	129 N	156 CD	9.714
129 N	154 CB	9.781	129 N	156 NE	9.846
129 N	60 O	9.947	129 N	154 CG2	10.079
129 N	38 CD2	10.174	129 N	61 C	10.212
129 N	38 CD1	10.521	129 N	132 CG2	10.557
129 N	60 OD2	10.755	129 N	154 CG1	10.857
129 N	132 CA	10.861	129 N	61 O	10.904
129 N	38 CG	10.956	129 N	154 CD1	11.002
129 N	156 CZ	11.059	129 N	132 OG1	11.066
129 N	38 CB	11.126	129 N	38 O	11.147
129 N	132 CB	11.227	129 N	156 NH2	11.334
129 N	38 CA	11.810	129 N	38 C	11.929
129 N	132 C	11.992	129 CA	128 C	2.374
129 CA	130 N	2.377	129 CA	128 O	2.683
129 CA	301 OH2	3.560	129 CA	300 OH2	3.614
129 CA	128 CA	3.704	129 CA	130 CA	3.762
129 CA	150 O	3.819	129 CA	128 CB	4.163
129 CA	130 C	4.480	129 CA	150 N	4.525
129 CA	130 O	4.654	129 CA	128 N	4.722
129 CA	130 CB	4.788	129 CA	150 C	4.807
129 CA	61 CE1	4.829	129 CA	152 SG	4.909
129 CA	128 CG2	4.997	129 CA	61 NE2	5.014
129 CA	150 CB	5.055	129 CA	150 CA	5.071
129 CA	128 CG1	5.243	129 CA	131 N	5.353
129 CA	155 CA	5.416	129 CA	149 CA	5.433
129 CA	149 C	5.524	129 CA	127 C	5.613
129 CA	149 CB	5.682	129 CA	157 NH2	5.711
129 CA	127 O	5.801	129 CA	156 N	5.887
129 CA	27 O	5.894	129 CA	61 ND1	5.927
129 CA	131 OG	5.955	129 CA	27 CD1	5.969
129 CA	151 N	6.019	129 CA	148 O	6.058
129 CA	61 CD2	6.221	129 CA	130 CG	6.223
129 CA	155 C	6.257	129 CA	152 CB	6.273
129 CA	131 CA	6.439	129 CA	155 N	6.459
129 CA	151 CA	6.468	129 CA	157 NE	6.488
129 CA	127 CB	6.496	129 CA	149 CG2	6.569

Fig. 8C

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CA	152 N	6.588	129 CA	151 C	6.596
129 CA	149 CG1	6.605	129 CA	27 CA	6.653
129 CA	157 CZ	6.668	129 CA	149 N	6.683
129 CA	149 O	6.685	129 CA	61 CG	6.713
129 CA	27 CG	6.715	129 CA	27 C	6.727
129 CA	130 CD1	6.748	129 CA	157 N	6.753
129 CA	127 CA	6.762	129 CA	131 CB	6.857
129 CA	148 C	6.859	129 CA	157 CB	6.963
129 CA	27 CB	7.013	129 CA	151 O	7.040
129 CA	156 CA	7.066	129 CA	152 CA	7.159
129 CA	156 CB	7.216	129 CA	130 CD2	7.220
129 CA	157 CG	7.229	129 CA	154 O	7.266
129 CA	154 C	7.272	129 CA	156 CG	7.398
129 CA	155 O	7.453	129 CA	156 C	7.522
129 CA	157 CA	7.530	129 CA	157 CD	7.534
129 CA	157 O	7.608	129 CA	131 C	7.706
129 CA	148 ND1	7.706	129 CA	151 CD1	7.730
129 CA	127 OG	7.739	129 CA	157 NH1	7.809
129 CA	27 N	7.855	129 CA	152 C	7.883
129 CA	148 CE1	7.907	129 CA	151 CB	7.924
129 CA	152 O	7.986	129 CA	61 N	7.986
129 CA	157 C	8.036	129 CA	127 N	8.061
129 CA	61 CB	8.064	129 CA	131 O	8.123
129 CA	27 CD2	8.130	129 CA	148 CA	8.359
129 CA	61 CA	8.429	129 CA	60 CA	8.460
129 CA	154 CA	8.491	129 CA	132 N	8.508
129 CA	151 CG	8.533	129 CA	148 CG	8.540
129 CA	60 N	8.570	129 CA	156 CD	8.594
129 CA	156 NE	8.600	129 CA	154 N	8.612
129 CA	156 O	8.710	129 CA	60 C	8.740
129 CA	148 NE2	8.803	129 CA	148 N	8.804
129 CA	60 OD1	8.811	129 CA	38 CD2	8.831
129 CA	148 CB	8.920	129 CA	148 CD2	9.180
129 CA	38 CD1	9.319	129 CA	132 CG2	9.573
129 CA	60 CG	9.635	129 CA	60 CB	9.635
129 CA	38 CG	9.687	129 CA	156 CZ	9.775
129 CA	60 O	9.795	129 CA	132 CA	9.825
129 CA	154 CB	9.837	129 CA	151 CD2	9.841
129 CA	132 OG1	9.875	129 CA	38 CB	9.925
129 CA	61 C	9.938	129 CA	156 NH2	9.982
129 CA	154 CG2	10.014	129 CA	38 O	10.059
129 CA	132 CB	10.149	129 CA	61 O	10.529
129 CA	38 CA	10.583	129 CA	60 OD2	10.652
129 CA	38 C	10.796	129 CA	132 O	10.863
129 CA	156 NH1	10.881	129 CA	132 C	10.911
129 CA	154 CG1	11.054	129 CA	154 CD1	11.303

Fig. 8D

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CA	38 N	11.864	129 C	130 N	1.324
129 C	130 CA	2.432	129 C	130 C	3.200
129 C	128 C	3.511	129 C	130 O	3.653
129 C	130 CB	3.668	129 C	301 OH2	3.711
129 C	150 N	3.953	129 C	131 N	3.970
129 C	128 O	4.002	129 C	150 O	4.219
129 C	149 CA	4.353	129 C	61 NE2	4.438
129 C	128 CA	4.606	129 C	148 O	4.620
129 C	61 CE1	4.633	129 C	300 OH2	4.672
129 C	128 CB	4.685	129 C	149 C	4.723
129 C	149 CB	4.759	129 C	150 CA	4.842
129 C	150 CB	4.879	129 C	131 OG	4.900
129 C	150 C	4.982	129 C	130 CG	4.985
129 C	131 CA	5.168	129 C	157 NH2	5.225
129 C	130 CD1	5.394	129 C	149 N	5.463
129 C	27 CD1	5.482	129 C	148 C	5.493
129 C	149 CG1	5.529	129 C	128 CG1	5.535
129 C	128 CG2	5.606	129 C	131 CB	5.637
129 C	61 CD2	5.640	129 C	128 N	5.842
129 C	61 ND1	5.846	129 C	149 CG2	5.875
129 C	27 O	5.915	129 C	149 O	5.940
129 C	27 CG	6.060	129 C	130 CD2	6.144
129 C	152 SG	6.169	129 C	151 N	6.282
129 C	157 CZ	6.326	129 C	131 C	6.371
129 C	157 NE	6.393	129 C	61 CG	6.403
129 C	27 CA	6.522	129 C	27 CB	6.554
129 C	148 ND1	6.607	129 C	131 O	6.700
129 C	27 C	6.709	129 C	127 C	6.768
129 C	127 O	6.836	129 C	155 CA	6.840
129 C	148 CE1	6.889	129 C	148 CA	6.974
129 C	151 CA	6.999	129 C	156 N	7.050
129 C	132 N	7.269	129 C	148 CG	7.302
129 C	151 C	7.308	129 C	152 CB	7.345
129 C	148 N	7.351	129 C	27 CD2	7.397
129 C	157 NH1	7.416	129 C	152 N	7.532
129 C	157 CB	7.551	129 C	155 C	7.573
129 C	157 CG	7.595	129 C	157 CD	7.629
129 C	148 CB	7.629	129 C	151 O	7.647
129 C	157 N	7.668	129 C	148 NE2	7.689
129 C	61 CB	7.818	129 C	27 N	7.826
129 C	127 CB	7.899	129 C	155 N	7.930
129 C	148 CD2	7.937	129 C	61 N	7.951
129 C	151 CD1	7.962	129 C	127 CA	8.030
129 C	156 CB	8.055	129 C	156 CA	8.093
129 C	61 CA	8.168	129 C	152 CA	8.207
129 C	156 CG	8.265	129 C	157 CA	8.333

Fig. 8E

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C	151 CB	8.379	129 C	132 CG2	8.406
129 C	156 C	8.469	129 C	132 CA	8.559
129 C	154 O	8.638	129 C	157 O	8.695
129 C	154 C	8.717	129 C	155 O	8.785
129 C	60 CA	8.818	129 C	132 OG1	8.844
129 C	60 N	8.870	129 C	60 C	8.886
129 C	38 CD2	8.894	129 C	151 CG	8.903
129 C	157 C	8.977	129 C	132 CB	8.980
129 C	152 C	9.078	129 C	156 NE	9.117
129 C	127 OG	9.169	129 C	152 O	9.204
129 C	127 N	9.307	129 C	156 CD	9.324
129 C	60 OD1	9.557	129 C	156 O	9.606
129 C	61 C	9.617	129 C	132 C	9.671
129 C	132 O	9.711	129 C	38 CD1	9.761
129 C	38 O	9.885	129 C	38 CG	9.905
129 C	60 O	9.926	129 C	154 CA	9.956
129 C	154 N	10.032	129 C	61 O	10.072
129 C	151 CD2	10.085	129 C	38 CB	10.089
129 C	60 CB	10.129	129 C	156 CZ	10.197
129 C	156 NH2	10.217	129 C	60 CG	10.247
129 C	38 CA	10.543	129 C	38 C	10.704
129 C	60 OD2	11.226	129 C	154 CB	11.291
129 C	156 NH1	11.392	129 C	154 CG2	11.463
129 C	38 N	11.821	129 O	130 N	2.240
129 O	130 CA	2.765	129 O	150 N	2.876
129 O	149 CA	3.368	129 O	130 C	3.377
129 O	149 C	3.617	129 O	131 N	3.740
129 O	61 NE2	3.757	129 O	150 O	3.782
129 O	148 O	3.794	129 O	150 CA	3.863
129 O	150 CB	3.935	129 O	149 CB	4.061
129 O	130 O	4.080	129 O	128 C	4.129
129 O	130 CB	4.162	129 O	61 CE1	4.210
129 O	150 C	4.288	129 O	131 OG	4.342
129 O	149 N	4.450	129 O	148 C	4.546
129 O	61 CD2	4.800	129 O	149 O	4.817
129 O	128 O	4.847	129 O	301 OH2	4.903
129 O	131 CA	4.926	129 O	149 CG1	4.965
129 O	128 CA	4.980	129 O	128 CB	5.074
129 O	131 CB	5.121	129 O	149 CG2	5.142
129 O	130 CG	5.257	129 O	61 ND1	5.343
129 O	130 CD1	5.363	129 O	148 ND1	5.464
129 O	151 N	5.605	129 O	128 CG1	5.635
129 O	61 CG	5.673	129 O	148 CE1	5.821
129 O	300 OH2	5.825	129 O	27 CD1	5.839
129 O	148 CA	6.030	129 O	157 NH2	6.102
129 O	131 C	6.158	129 O	128 CG2	6.205

Fig. 8F

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O	148 CG	6.215	129 O	128 N	6.322
129 O	152 SG	6.359	129 O	131 O	6.380
129 O	27 CG	6.483	129 O	151 CA	6.526
129 O	148 N	6.542	129 O	148 CB	6.556
129 O	130 CD2	6.578	129 O	148 NE2	6.696
129 O	151 C	6.910	129 O	148 CD2	6.929
129 O	127 O	6.966	129 O	27 O	6.969
129 O	61 CB	7.037	129 O	61 N	7.095
129 O	127 C	7.108	129 O	151 O	7.131
129 O	132 N	7.198	129 O	27 CB	7.206
129 O	61 CA	7.252	129 O	157 CZ	7.276
129 O	152 CB	7.282	129 O	27 CA	7.326
129 O	152 N	7.342	129 O	151 CD1	7.461
129 O	157 NE	7.470	129 O	155 CA	7.649
129 O	27 C	7.678	129 O	27 CD2	7.690
129 O	151 CB	7.841	129 O	156 N	7.999
129 O	152 CA	8.085	129 O	60 N	8.114
129 O	60 C	8.122	129 O	60 CA	8.145
129 O	157 NH1	8.292	129 O	151 CG	8.388
129 O	127 CB	8.456	129 O	155 C	8.474
129 O	127 CA	8.475	129 O	132 CA	8.500
129 O	27 N	8.596	129 O	132 CG2	8.645
129 O	155 N	8.657	129 O	61 C	8.659
129 O	157 CD	8.753	129 O	157 CG	8.758
129 O	157 CB	8.761	129 O	157 N	8.815
129 O	156 CB	8.954	129 O	156 CG	9.014
129 O	156 CA	9.075	129 O	132 OG1	9.090
129 O	61 O	9.099	129 O	152 C	9.115
129 O	132 CB	9.119	129 O	154 O	9.171
129 O	60 O	9.175	129 O	60 OD1	9.237
129 O	152 O	9.302	129 O	154 C	9.325
129 O	151 CD2	9.450	129 O	157 CA	9.528
129 O	132 C	9.531	129 O	60 CB	9.539
129 O	156 C	9.557	129 O	132 O	9.585
129 O	127 N	9.643	129 O	155 O	9.693
129 O	38 CD2	9.736	129 O	156 NE	9.775
129 O	127 OG	9.787	129 O	60 CG	9.799
129 O	157 O	9.857	129 O	156 CD	9.999
129 O	157 C	10.173	129 O	154 N	10.438
129 O	154 CA	10.519	129 O	156 O	10.702
129 O	38 CD1	10.736	129 O	60 OD2	10.775
129 O	156 NH2	10.835	129 O	38 CG	10.838
129 O	156 CZ	10.849	129 O	38 O	10.865
129 O	38 CB	11.090	129 O	38 CA	11.485
129 O	38 C	11.687	129 O	154 CB	11.882
129 CB	128 C	3.142	129 CB	128 O	3.361

Fig. 8G

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CB	130 N	3.507	129 CB	150 O	3.681
129 CB	61 CE1	3.735	129 CB	152 SG	4.007
129 CB	300 OH2	4.159	129 CB	61 NE2	4.230
129 CB	150 CB	4.342	129 CB	128 CA	4.389
129 CB	150 C	4.513	129 CB	150 N	4.577
129 CB	61 ND1	4.692	129 CB	301 OH2	4.693
129 CB	150 CA	4.745	129 CB	130 CA	4.754
129 CB	155 CA	4.947	129 CB	130 C	5.107
129 CB	130 O	5.155	129 CB	152 CB	5.205
129 CB	128 N	5.215	129 CB	128 CB	5.218
129 CB	61 CD2	5.382	129 CB	156 N	5.510
129 CB	61 CG	5.624	129 CB	151 N	5.682
129 CB	131 OG	5.683	129 CB	149 C	5.764
129 CB	131 N	5.810	129 CB	127 C	5.819
129 CB	155 C	5.832	129 CB	127 O	5.856
129 CB	152 N	5.957	129 CB	155 N	5.959
129 CB	151 C	5.968	129 CB	130 CB	5.970
129 CB	149 CA	5.994	129 CB	128 CG2	6.143
129 CB	151 CA	6.158	129 CB	128 CG1	6.194
129 CB	151 O	6.218	129 CB	152 CA	6.291
129 CB	154 O	6.324	129 CB	157 NH2	6.420
129 CB	127 CB	6.441	129 CB	149 CB	6.513
129 CB	154 C	6.540	129 CB	148 O	6.565
129 CB	156 CG	6.633	129 CB	131 CA	6.662
129 CB	156 CA	6.739	129 CB	156 CB	6.749
129 CB	131 CB	6.813	129 CB	149 O	6.817
129 CB	61 N	6.859	129 CB	127 CA	6.888
129 CB	61 CB	6.911	129 CB	157 N	6.955
129 CB	155 O	7.041	129 CB	152 C	7.124
129 CB	149 N	7.181	129 CB	27 O	7.249
129 CB	60 CA	7.252	129 CB	149 CG2	7.281
129 CB	130 CG	7.308	129 CB	157 NE	7.333
129 CB	148 C	7.339	129 CB	61 CA	7.361
129 CB	27 CD1	7.419	129 CB	60 OD1	7.420
129 CB	157 CZ	7.427	129 CB	152 O	7.439
129 CB	156 C	7.488	129 CB	60 C	7.512
129 CB	148 CE1	7.517	129 CB	148 ND1	7.519
129 CB	60 N	7.545	129 CB	149 CG1	7.584
129 CB	157 CB	7.619	129 CB	127 OG	7.662
129 CB	151 CB	7.668	129 CB	156 CD	7.767
129 CB	157 CG	7.814	129 CB	154 CA	7.816
129 CB	130 CD1	7.817	129 CB	154 N	7.821
129 CB	156 NE	7.870	129 CB	151 CD1	7.948
129 CB	157 CA	7.963	129 CB	157 O	8.030
129 CB	127 N	8.051	129 CB	131 C	8.082
129 CB	27 CA	8.140	129 CB	27 C	8.144

Fig. 8H

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CB	27 CG	8.188	129 CB	60 CG	8.257
129 CB	157 CD	8.312	129 CB	60 CB	8.367
129 CB	130 CD2	8.407	129 CB	157 NH1	8.444
129 CB	148 NE2	8.478	129 CB	27 CB	8.511
129 CB	60 O	8.514	129 CB	148 CG	8.521
129 CB	151 CG	8.522	129 CB	157 C	8.524
129 CB	131 O	8.620	129 CB	156 O	8.689
129 CB	148 CA	8.779	129 CB	38 CD2	8.803
129 CB	132 N	8.846	129 CB	61 C	8.888
129 CB	148 CD2	9.064	129 CB	156 CZ	9.099
129 CB	154 CB	9.107	129 CB	148 CB	9.113
129 CB	60 OD2	9.231	129 CB	38 CD1	9.233
129 CB	148 N	9.233	129 CB	27 N	9.325
129 CB	154 CG2	9.394	129 CB	156 NH2	9.399
129 CB	61 O	9.534	129 CB	27 CD2	9.583
129 CB	38 CG	9.702	129 CB	151 CD2	9.793
129 CB	38 CB	10.167	129 CB	156 NH1	10.170
129 CB	132 CA	10.250	129 CB	132 OG1	10.284
129 CB	132 CG2	10.292	129 CB	154 CG1	10.374
129 CB	132 CB	10.674	129 CB	38 O	10.707
129 CB	154 CD1	10.812	129 CB	38 CA	10.912
129 CB	132 O	10.976	129 CB	132 C	11.176
129 CB	38 C	11.323	129 OG	61 CE1	2.985
129 OG	130 N	3.571	129 OG	61 NE2	3.623
129 OG	61 ND1	4.074	129 OG	130 O	4.381
129 OG	300 OH2	4.388	129 OG	128 C	4.417
129 OG	128 O	4.440	129 OG	130 C	4.578
129 OG	130 CA	4.638	129 OG	301 OH2	4.714
129 OG	150 CB	4.840	129 OG	131 OG	4.860
129 OG	61 CD2	4.897	129 OG	150 O	4.925
129 OG	152 SG	4.971	129 OG	61 CG	5.124
129 OG	131 N	5.263	129 OG	156 N	5.282
129 OG	155 CA	5.306	129 OG	150 N	5.308
129 OG	150 CA	5.536	129 OG	150 C	5.597
129 OG	157 NH2	5.711	129 OG	128 CA	5.747
129 OG	156 CG	5.853	129 OG	131 CA	5.863
129 OG	155 C	5.877	129 OG	130 CB	5.894
129 OG	131 CB	6.013	129 OG	156 CB	6.014
129 OG	152 CB	6.043	129 OG	156 CA	6.303
129 OG	149 C	6.418	129 OG	128 CB	6.467
129 OG	155 N	6.487	129 OG	61 CB	6.497
129 OG	148 O	6.525	129 OG	149 CA	6.534
129 OG	128 N	6.543	129 OG	154 O	6.605
129 OG	157 N	6.702	129 OG	156 NE	6.752
129 OG	157 CZ	6.766	129 OG	151 N	6.795
129 OG	156 CD	6.827	129 OG	157 NE	6.850

Fig. 8I

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 OG	61 N	6.950	129 OG	154 C	7.003
129 OG	155 O	7.100	129 OG	130 CG	7.102
129 OG	156 C	7.104	129 OG	151 C	7.105
129 OG	152 N	7.130	129 OG	127 C	7.171
129 OG	151 O	7.182	129 OG	148 CE1	7.194
129 OG	61 CA	7.220	129 OG	127 O	7.243
129 OG	149 CB	7.249	129 OG	152 CA	7.293
129 OG	128 CG2	7.305	129 OG	131 C	7.327
129 OG	157 CG	7.348	129 OG	151 CA	7.395
129 OG	148 ND1	7.400	129 OG	157 CB	7.410
129 OG	148 C	7.443	129 OG	149 O	7.473
129 OG	128 CG1	7.476	129 OG	27 O	7.516
129 OG	149 N	7.529	129 OG	127 CB	7.558
129 OG	60 CA	7.627	129 OG	157 NH1	7.635
129 OG	60 C	7.640	129 OG	60 OD1	7.674
129 OG	38 CD2	7.680	129 OG	130 CD1	7.756
129 OG	157 CA	7.766	129 OG	157 CD	7.848
129 OG	156 CZ	7.927	129 OG	132 N	7.952
129 OG	148 NE2	8.010	129 OG	131 O	8.029
129 OG	60 N	8.128	129 OG	156 NH2	8.135
129 OG	152 C	8.147	129 OG	127 CA	8.153
129 OG	27 CD1	8.158	129 OG	149 CG2	8.177
129 OG	149 CG1	8.186	129 OG	130 CD2	8.220
129 OG	157 O	8.222	129 OG	156 O	8.247
129 OG	38 CD1	8.312	129 OG	148 CG	8.355
129 OG	154 CA	8.409	129 OG	60 CG	8.473
129 OG	154 N	8.509	129 OG	60 O	8.509
129 OG	27 C	8.533	129 OG	157 C	8.558
129 OG	152 O	8.578	129 OG	127 OG	8.685
129 OG	38 CG	8.688	129 OG	148 CD2	8.695
129 OG	27 CA	8.704	129 OG	61 C	8.709
129 OG	27 CG	8.716	129 OG	60 CB	8.727
129 OG	148 CA	8.787	129 OG	151 CB	8.895
129 OG	27 CB	8.971	129 OG	148 N	9.033
129 OG	156 NH1	9.061	129 OG	148 CB	9.111
129 OG	61 O	9.220	129 OG	151 CD1	9.245
129 OG	38 CB	9.268	129 OG	132 OG1	9.277
129 OG	60 OD2	9.309	129 OG	127 N	9.321
129 OG	132 CA	9.386	129 OG	154 CB	9.551
129 OG	132 CG2	9.557	129 OG	154 CG2	9.724
129 OG	132 CB	9.791	129 OG	151 CG	9.810
129 OG	132 O	9.908	129 OG	38 O	9.961
129 OG	38 CA	9.965	129 OG	27 N	9.985
129 OG	27 CD2	10.115	129 OG	132 C	10.215
129 OG	38 C	10.504	129 OG	154 CG1	10.921
129 OG	151 CD2	11.021	129 OG	38 N	11.065

Fig. 8J

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 OG	154 CD1	11.458	129 P1	61 CE1	3.821
129 P1	156 N	4.026	129 P1	300 OH2	4.041
129 P1	156 CG	4.281	129 P1	156 CB	4.476
129 P1	155 CA	4.568	129 P1	130 N	4.598
129 P1	61 ND1	4.712	129 P1	61 NE2	4.721
129 P1	155 C	4.796	129 P1	301 OH2	4.892
129 P1	128 O	4.895	129 P1	156 CA	4.896
129 P1	130 O	4.931	129 P1	128 C	5.235
129 P1	156 NE	5.255	129 P1	156 CD	5.271
129 P1	152 SG	5.281	129 P1	130 C	5.464
129 P1	157 N	5.627	129 P1	157 NH2	5.639
129 P1	130 CA	5.683	129 P1	131 OG	5.794
129 P1	156 C	5.818	129 P1	154 O	5.856
129 P1	155 N	5.868	129 P1	61 CD2	5.946
129 P1	61 CG	5.951	129 P1	155 O	5.980
129 P1	150 CB	6.225	129 P1	150 O	6.244
129 P1	131 N	6.264	129 P1	154 C	6.349
129 P1	152 CB	6.428	129 P1	156 CZ	6.474
129 P1	157 CZ	6.515	129 P1	157 NE	6.522
129 P1	157 CG	6.564	129 P1	38 CD2	6.582
129 P1	128 CA	6.645	129 P1	131 CA	6.656
129 P1	157 CB	6.687	129 P1	130 CB	6.752
129 P1	156 NH2	6.805	129 P1	157 CA	6.826
129 P1	150 N	6.878	129 P1	131 CB	6.898
129 P1	156 O	6.919	129 P1	38 CD1	6.961
129 P1	150 C	6.968	129 P1	150 CA	7.018
129 P1	128 N	7.175	129 P1	61 CB	7.235
129 P1	157 NH1	7.262	129 P1	157 CD	7.301
129 P1	157 O	7.439	129 P1	128 CB	7.449
129 P1	38 CG	7.480	129 P1	156 NH1	7.561
129 P1	127 CB	7.661	129 P1	157 C	7.716
129 P1	27 O	7.767	129 P1	127 C	7.776
129 P1	152 CA	7.796	129 P1	154 CA	7.857
129 P1	60 OD1	7.879	129 P1	152 N	7.879
129 P1	61 N	7.885	129 P1	148 O	7.905
129 P1	130 CG	7.944	129 P1	149 C	8.001
129 P1	127 O	8.005	129 P1	151 C	8.058
129 P1	128 CG2	8.072	129 P1	131 C	8.072
129 P1	151 N	8.088	129 P1	149 CA	8.090
129 P1	151 O	8.125	129 P1	61 CA	8.152
129 P1	154 N	8.154	129 P1	38 CB	8.197
129 P1	60 CA	8.381	129 P1	60 C	8.408
129 P1	148 CE1	8.425	129 P1	152 C	8.461
129 P1	132 N	8.474	129 P1	127 CA	8.514
129 P1	151 CA	8.534	129 P1	127 OG	8.602
129 P1	128 CG1	8.608	129 P1	149 CB	8.760

Fig. 8K

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 P1	148 ND1	8.772	129 P1	60 CG	8.784
129 P1	130 CD1	8.807	129 P1	154 CB	8.815
129 P1	154 CG2	8.819	129 P1	27 C	8.879
129 P1	148 C	8.895	129 P1	130 CD2	8.902
129 P1	131 O	8.923	129 P1	152 O	8.941
129 P1	38 CA	9.042	129 P1	149 O	9.048
129 P1	149 N	9.061	129 P1	60 N	9.070
129 P1	148 NE2	9.144	129 P1	60 O	9.149
129 P1	27 CD1	9.198	129 P1	60 CB	9.293
129 P1	27 CA	9.299	129 P1	38 O	9.334
129 P1	132 OG1	9.399	129 P1	60 OD2	9.509
129 P1	61 C	9.598	129 P1	149 CG1	9.639
129 P1	27 CG	9.659	129 P1	127 N	9.685
129 P1	27 CB	9.696	129 P1	149 CG2	9.705
129 P1	148 CG	9.706	129 P1	38 C	9.723
129 P1	132 CA	9.881	129 P1	148 CD2	9.911
129 P1	132 CG2	9.949	129 P1	151 CB	10.049
129 P1	38 N	10.063	129 P1	61 O	10.087
129 P1	132 CB	10.118	129 P1	148 CA	10.198
129 P1	132 O	10.216	129 P1	154 CG1	10.271
129 P1	148 N	10.316	129 P1	151 CD1	10.537
129 P1	148 CB	10.538	129 P1	27 N	10.558
129 P1	132 C	10.643	129 P1	154 CD1	10.859
129 P1	151 CG	11.019	129 P1	27 CD2	11.105
129 O3	156 CG	3.793	129 O3	156 N	3.878
129 O3	155 CA	4.039	129 O3	61 CE1	4.090
129 O3	155 C	4.345	129 O3	156 CB	4.469
129 O3	152 SG	4.522	129 O3	61 ND1	4.562
129 O3	154 O	4.585	129 O3	156 CD	4.779
129 O3	156 CA	4.837	129 O3	300 OH2	4.883
129 O3	155 N	5.127	129 O3	156 NE	5.139
129 O3	61 NE2	5.260	129 O3	154 C	5.296
129 O3	128 O	5.415	129 O3	155 O	5.423
129 O3	152 CB	5.450	129 O3	128 C	5.777
129 O3	61 CG	5.917	129 O3	130 N	6.035
129 O3	156 C	6.077	129 O3	157 N	6.144
129 O3	61 CD2	6.262	129 O3	301 OH2	6.293
129 O3	150 CB	6.340	129 O3	150 O	6.438
129 O3	156 CZ	6.439	129 O3	130 O	6.505
129 O3	60 OD1	6.598	129 O3	154 CA	6.785
129 O3	131 OG	6.796	129 O3	152 CA	6.910
129 O3	61 CB	6.970	129 O3	130 C	6.981
129 O3	154 N	6.985	129 O3	156 NH2	7.024
129 O3	128 CA	7.048	129 O3	150 C	7.076
129 O3	156 O	7.151	129 O3	130 CA	7.170
129 O3	157 NH2	7.223	129 O3	150 CA	7.272

Fig. 8L

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O3	127 CB	7.276	129 O3	152 N	7.276
129 O3	156 NH1	7.349	129 O3	128 N	7.354
129 O3	61 N	7.442	129 O3	150 N	7.448
129 O3	38 CD2	7.493	129 O3	157 CA	7.495
129 O3	152 C	7.516	129 O3	38 CD1	7.523
129 O3	151 O	7.538	129 O3	151 C	7.575
129 O3	60 CA	7.575	129 O3	60 CG	7.582
129 O3	154 CB	7.645	129 O3	157 CB	7.651
129 O3	157 CG	7.664	129 O3	131 N	7.672
129 O3	127 C	7.696	129 O3	60 C	7.719
129 O3	154 CG2	7.779	129 O3	157 O	7.802
129 O3	127 O	7.853	129 O3	61 CA	7.882
129 O3	157 NE	7.960	129 O3	131 CA	8.001
129 O3	151 N	8.022	129 O3	131 CB	8.031
129 O3	157 CZ	8.032	129 O3	128 CB	8.108
129 O3	127 OG	8.116	129 O3	152 O	8.144
129 O3	157 C	8.238	129 O3	60 OD2	8.253
129 O3	38 CG	8.260	129 O3	127 CA	8.272
129 O3	60 CB	8.275	129 O3	130 CB	8.299
129 O3	151 CA	8.324	129 O3	60 O	8.377
129 O3	60 N	8.418	129 O3	157 CD	8.592
129 O3	149 C	8.677	129 O3	157 NH1	8.731
129 O3	128 CG2	8.766	129 O3	149 CA	9.017
129 O3	148 CE1	9.022	129 O3	148 O	9.086
129 O3	27 O	9.087	129 O3	154 CG1	9.109
129 O3	38 CB	9.137	129 O3	128 CG1	9.214
129 O3	127 N	9.270	129 O3	61 C	9.294
129 O3	148 ND1	9.458	129 O3	131 C	9.469
129 O3	130 CG	9.516	129 O3	149 O	9.612
129 O3	149 CB	9.717	129 O3	151 CB	9.806
129 O3	148 NE2	9.830	129 O3	154 CD1	9.862
129 O3	132 N	9.880	129 O3	61 O	9.898
129 O3	148 C	9.977	129 O3	149 N	10.032
129 O3	38 CA	10.119	129 O3	27 C	10.167
129 O3	130 CD1	10.306	129 O3	131 O	10.325
129 O3	27 CD1	10.407	129 O3	149 CG2	10.491
129 O3	130 CD2	10.504	129 O3	148 CG	10.528
129 O3	27 CA	10.558	129 O3	38 O	10.635
129 O3	151 CD1	10.659	129 O3	148 CD2	10.731
129 O3	149 CG1	10.746	129 O3	132 OG1	10.842
129 O3	38 C	10.911	129 O3	151 CG	10.924
129 O3	27 CG	11.008	129 O3	38 N	11.034
129 O3	27 CB	11.065	129 O3	148 CA	11.269
129 O3	132 CA	11.309	129 O3	148 CB	11.440
129 O3	132 O	11.452	129 O3	148 N	11.488
129 O3	132 CG2	11.516	129 O3	132 CB	11.605

Fig. 8M

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O3	27 N	11.739	129 O3	132 C	11.968
129 O4	61 CE1	3.831	129 O4	156 CG	4.254
129 O4	156 NE	4.418	129 O4	156 CB	4.454
129 O4	130 O	4.456	129 O4	61 NE2	4.644
129 O4	61 ND1	4.718	129 O4	156 CD	4.845
129 O4	156 N	4.853	129 O4	130 N	5.075
129 O4	300 OH2	5.108	129 O4	157 NH2	5.184
129 O4	131 OG	5.209	129 O4	130 C	5.216
129 O4	156 CA	5.312	129 O4	301 OH2	5.444
129 O4	156 CZ	5.479	129 O4	38 CD2	5.523
129 O4	156 NH2	5.578	129 O4	61 CD2	5.838
129 O4	130 CA	5.839	129 O4	155 C	5.852
129 O4	61 CG	5.885	129 O4	131 N	5.901
129 O4	155 CA	5.921	129 O4	131 CA	5.951
129 O4	157 CZ	6.077	129 O4	157 N	6.107
129 O4	156 C	6.160	129 O4	131 CB	6.198
129 O4	38 CD1	6.333	129 O4	128 O	6.343
129 O4	157 NE	6.361	129 O4	157 CG	6.537
129 O4	157 NH1	6.570	129 O4	38 CG	6.622
129 O4	128 C	6.656	129 O4	156 NH1	6.692
129 O4	152 SG	6.795	129 O4	130 CB	6.864
129 O4	155 O	6.949	129 O4	150 CB	6.960
129 O4	157 CB	7.013	129 O4	154 O	7.062
129 O4	156 O	7.102	129 O4	157 CD	7.162
129 O4	61 CB	7.178	129 O4	157 CA	7.235
129 O4	155 N	7.253	129 O4	131 C	7.311
129 O4	38 CB	7.477	129 O4	150 O	7.490
129 O4	132 N	7.516	129 O4	150 N	7.655
129 O4	154 C	7.670	129 O4	152 CB	7.789
129 O4	130 CG	7.827	129 O4	150 CA	7.892
129 O4	148 O	7.931	129 O4	128 CA	8.086
129 O4	150 C	8.096	129 O4	38 CA	8.180
129 O4	148 CE1	8.218	129 O4	132 OG1	8.266
129 O4	157 O	8.291	129 O4	131 O	8.306
129 O4	61 CA	8.307	129 O4	61 N	8.314
129 O4	27 O	8.327	129 O4	157 C	8.360
129 O4	149 CA	8.632	129 O4	149 C	8.663
129 O4	38 O	8.704	129 O4	60 OD1	8.707
129 O4	128 N	8.708	129 O4	148 ND1	8.730
129 O4	148 NE2	8.732	129 O4	128 CB	8.754
129 O4	130 CD1	8.774	129 O4	130 CD2	8.776
129 O4	132 CA	8.901	129 O4	60 C	8.905
129 O4	132 O	8.979	129 O4	148 C	9.009
129 O4	38 C	9.010	129 O4	38 N	9.081
129 O4	132 CB	9.113	129 O4	132 CG2	9.137
129 O4	60 CA	9.138	129 O4	152 CA	9.204

Fig. 8N

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O4	154 CA	9.206	129 O4	127 CB	9.250
129 O4	151 N	9.263	129 O4	152 N	9.321
129 O4	151 O	9.339	129 O4	127 C	9.355
129 O4	128 CG2	9.369	129 O4	151 C	9.396
129 O4	149 N	9.397	129 O4	149 CB	9.453
129 O4	27 C	9.496	129 O4	60 CG	9.502
129 O4	60 O	9.507	129 O4	132 C	9.523
129 O4	154 N	9.540	129 O4	148 CD2	9.545
129 O4	148 CG	9.553	129 O4	127 O	9.562
129 O4	61 C	9.650	129 O4	149 O	9.696
129 O4	151 CA	9.859	129 O4	128 CG1	9.886
129 O4	154 CG2	9.932	129 O4	152 C	9.937
129 O4	60 N	9.938	129 O4	61 O	9.955
129 O4	27 CD1	9.975	129 O4	27 CA	10.020
129 O4	154 CB	10.025	129 O4	60 CB	10.065
129 O4	148 N	10.067	129 O4	60 OD2	10.078
129 O4	127 CA	10.114	129 O4	127 OG	10.153
129 O4	148 CA	10.168	129 O4	149 CG1	10.190
129 O4	27 CG	10.235	129 O4	27 CB	10.255
129 O4	152 O	10.480	129 O4	148 CB	10.502
129 O4	149 CG2	10.527	129 O4	127 N	11.292
129 O4	27 N	11.355	129 O4	151 CB	11.358
129 O4	154 CG1	11.523	129 O4	27 CD2	11.636
129 O4	151 CD1	11.823	129 O5	300 OH2	2.667
129 O5	156 N	3.025	129 O5	155 CA	3.821
129 O5	156 CB	3.849	129 O5	155 C	3.896
129 O5	301 OH2	3.902	129 O5	156 CA	3.938
129 O5	156 CG	4.108	129 O5	128 O	4.153
129 O5	157 N	4.258	129 O5	130 N	4.459
129 O5	156 C	4.627	129 O5	128 C	4.783
129 O5	130 O	5.092	129 O5	155 O	5.093
129 O5	157 NH2	5.124	129 O5	61 CE1	5.198
129 O5	155 N	5.239	129 O5	157 CB	5.290
129 O5	156 CD	5.325	129 O5	157 CG	5.334
129 O5	156 NE	5.388	129 O5	157 CA	5.413
129 O5	152 SG	5.481	129 O5	157 NE	5.543
129 O5	130 CA	5.686	129 O5	130 C	5.696
129 O5	154 O	5.732	129 O5	156 O	5.781
129 O5	157 CZ	5.796	129 O5	61 NE2	5.970
129 O5	154 C	5.981	129 O5	157 O	6.005
129 O5	61 ND1	6.148	129 O5	157 CD	6.178
129 O5	38 CD2	6.196	129 O5	128 CA	6.248
129 O5	38 CD1	6.257	129 O5	157 C	6.263
129 O5	130 CB	6.487	129 O5	156 CZ	6.591
129 O5	150 O	6.609	129 O5	128 N	6.627
129 O5	157 NH1	6.656	129 O5	27 O	6.670

Fig. 80

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O5	131 N	6.721	129 O5	131 OG	6.804
129 O5	38 CG	6.880	129 O5	152 CB	6.914
129 O5	128 CB	6.960	129 O5	156 NH2	6.975
129 O5	127 CB	7.065	129 O5	150 CB	7.193
129 O5	61 CD2	7.255	129 O5	131 CA	7.265
129 O5	128 CG2	7.330	129 O5	61 CG	7.356
129 O5	127 C	7.365	129 O5	38 CB	7.411
129 O5	154 CA	7.482	129 O5	150 N	7.493
129 O5	150 C	7.519	129 O5	156 NH1	7.612
129 O5	150 CA	7.759	129 O5	131 CB	7.763
129 O5	130 CG	7.783	129 O5	27 C	7.797
129 O5	127 O	7.812	129 O5	127 OG	7.913
129 O5	127 CA	7.973	129 O5	154 N	7.999
129 O5	152 CA	8.174	129 O5	152 N	8.193
129 O5	154 CG2	8.264	129 O5	128 CG1	8.268
129 O5	38 CA	8.356	129 O5	27 CA	8.359
129 O5	148 O	8.440	129 O5	154 CB	8.443
129 O5	38 O	8.493	129 O5	149 CA	8.523
129 O5	151 C	8.531	129 O5	130 CD2	8.536
129 O5	131 C	8.562	129 O5	149 C	8.582
129 O5	152 C	8.628	129 O5	151 N	8.629
129 O5	27 CD1	8.659	129 O5	61 CB	8.662
129 O5	130 CD1	8.779	129 O5	151 O	8.793
129 O5	60 OD1	8.862	129 O5	38 C	8.905
129 O5	132 N	8.913	129 O5	151 CA	8.913
129 O5	27 CB	8.914	129 O5	152 O	8.941
129 O5	149 CB	8.961	129 O5	27 CG	9.076
129 O5	61 N	9.158	129 O5	127 N	9.249
129 O5	131 O	9.372	129 O5	148 C	9.462
129 O5	38 N	9.477	129 O5	60 CA	9.490
129 O5	61 CA	9.506	129 O5	27 N	9.560
129 O5	132 OG1	9.561	129 O5	148 CE1	9.564
129 O5	149 N	9.587	129 O5	60 C	9.665
129 O5	149 O	9.701	129 O5	149 CG1	9.755
129 O5	148 ND1	9.781	129 O5	60 CG	9.859
129 O5	154 CG1	9.884	129 O5	149 CG2	9.927
129 O5	132 CG2	9.940	129 O5	60 N	10.076
129 O5	132 CA	10.242	129 O5	148 NE2	10.271
129 O5	132 CB	10.286	129 O5	154 CD1	10.295
129 O5	60 CB	10.367	129 O5	151 CB	10.430
129 O5	60 O	10.463	129 O5	27 CD2	10.559
129 O5	60 OD2	10.640	129 O5	148 CG	10.640
129 O5	151 CD1	10.713	129 O5	132 O	10.799
129 O5	148 CA	10.830	129 O5	148 CD2	10.920
129 O5	148 N	10.940	129 O5	61 C	10.978
129 O5	132 C	11.141	129 O5	151 CG	11.275

Fig. 8P

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O5	148 CB	11.334	129 O5	61 O	11.493
129 C5	61 CE1	3.704	129 C5	61 ND1	3.752
129 C5	156 CG	4.447	129 C5	152 SG	4.788
129 C5	154 O	4.895	129 C5	61 NE2	5.007
129 C5	155 CA	5.103	129 C5	156 CD	5.105
129 C5	156 N	5.117	129 C5	61 CG	5.119
129 C5	152 CB	5.235	129 C5	156 CB	5.446
129 C5	155 C	5.457	129 C5	156 NE	5.488
129 C5	60 OD1	5.543	129 C5	61 CD2	5.748
129 C5	154 C	5.823	129 C5	155 N	5.957
129 C5	61 CB	5.959	129 C5	156 CA	5.971
129 C5	150 CB	6.089	129 C5	300 OH2	6.321
129 C5	155 O	6.411	129 C5	60 CG	6.441
129 C5	61 N	6.514	129 C5	128 O	6.567
129 C5	60 CA	6.637	129 C5	60 C	6.662
129 C5	156 CZ	6.719	129 C5	150 O	6.745
129 C5	152 CA	6.749	129 C5	128 C	6.765
129 C5	131 OG	6.809	129 C5	61 CA	6.937
129 C5	60 OD2	6.996	129 C5	130 N	6.997
129 C5	150 C	7.160	129 C5	154 N	7.175
129 C5	60 O	7.186	129 C5	151 O	7.198
129 C5	154 CA	7.200	129 C5	150 CA	7.234
129 C5	60 CB	7.241	129 C5	152 N	7.277
129 C5	130 O	7.286	129 C5	156 NH2	7.311
129 C5	156 C	7.317	129 C5	151 C	7.466
129 C5	152 C	7.494	129 C5	157 N	7.509
129 C5	156 NH1	7.566	129 C5	301 OH2	7.619
129 C5	150 N	7.621	129 C5	60 N	7.660
129 C5	130 C	7.693	129 C5	128 CA	7.913
129 C5	154 CB	7.967	129 C5	151 N	8.000
129 C5	130 CA	8.011	129 C5	127 CB	8.056
129 C5	131 CB	8.130	129 C5	131 N	8.180
129 C5	128 N	8.248	129 C5	61 C	8.265
129 C5	154 CG2	8.275	129 C5	152 O	8.300
129 C5	157 NH2	8.322	129 C5	156 O	8.323
129 C5	38 CD2	8.340	129 C5	131 CA	8.360
129 C5	151 CA	8.374	129 C5	127 O	8.397
129 C5	127 C	8.420	129 C5	38 CD1	8.479
129 C5	148 CE1	8.660	129 C5	149 C	8.855
129 C5	61 O	8.883	129 C5	157 CA	8.887
129 C5	127 OG	8.894	129 C5	127 CA	9.016
129 C5	157 CG	9.020	129 C5	128 CB	9.048
129 C5	157 CB	9.077	129 C5	157 O	9.176
129 C5	38 CG	9.181	129 C5	157 CZ	9.204
129 C5	148 ND1	9.238	129 C5	157 NE	9.252
129 C5	130 CB	9.265	129 C5	149 CA	9.372

Fig. 8Q

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C5	154 CG1	9.387	129 C5	148 O	9.429
129 C5	148 NE2	9.480	129 C5	157 C	9.634
129 C5	149 O	9.660	129 C5	151 CB	9.789
129 C5	157 NH1	9.818	129 C5	128 CG2	9.846
129 C5	127 N	9.857	129 C5	131 C	9.868
129 C5	157 CD	9.924	129 C5	128 CG1	10.018
129 C5	38 CB	10.192	129 C5	149 CB	10.228
129 C5	148 C	10.240	129 C5	132 N	10.294
129 C5	149 N	10.295	129 C5	154 CD1	10.317
129 C5	148 CG	10.387	129 C5	130 CG	10.398
129 C5	27 O	10.444	129 C5	148 CD2	10.513
129 C5	131 O	10.734	129 C5	151 CD1	10.916
129 C5	149 CG2	10.919	129 C5	151 CG	11.036
129 C5	130 CD1	11.077	129 C5	38 CA	11.130
129 C5	149 CG1	11.330	129 C5	132 OG1	11.417
129 C5	148 CB	11.421	129 C5	148 CA	11.439
129 C5	27 CD1	11.442	129 C5	130 CD2	11.496
129 C5	27 C	11.512	129 C5	132 O	11.654
129 C5	148 N	11.685	129 C5	132 CA	11.746
129 C5	38 O	11.793	129 C5	27 CA	11.825
129 C5	38 N	11.940	129 C6	156 CG	3.825
129 C6	156 CD	4.164	129 C6	156 NE	4.733
129 C6	61 ND1	4.802	129 C6	154 O	4.864
129 C6	61 CE1	4.944	129 C6	156 CB	5.124
129 C6	156 N	5.239	129 C6	155 CA	5.536
129 C6	155 C	5.573	129 C6	156 CA	5.808
129 C6	152 SG	5.810	129 C6	60 OD1	5.892
129 C6	156 CZ	5.894	129 C6	154 C	5.953
129 C6	61 CG	6.123	129 C6	152 CB	6.129
129 C6	61 NE2	6.256	129 C6	155 N	6.285
129 C6	155 O	6.317	129 C6	156 NH1	6.557
129 C6	156 NH2	6.650	129 C6	61 CB	6.764
129 C6	60 CG	6.785	129 C6	61 CD2	6.892
129 C6	60 OD2	7.114	129 C6	300 OH2	7.169
129 C6	156 C	7.267	129 C6	154 CA	7.288
129 C6	154 N	7.357	129 C6	60 C	7.459
129 C6	60 CA	7.476	129 C6	61 N	7.489
129 C6	150 CB	7.514	129 C6	152 CA	7.633
129 C6	157 N	7.721	129 C6	128 O	7.747
129 C6	154 CB	7.763	129 C6	60 O	7.775
129 C6	60 CB	7.831	129 C6	61 CA	7.857
129 C6	131 OG	7.900	129 C6	154 CG2	7.978
129 C6	128 C	8.083	129 C6	156 O	8.125
129 C6	38 CD1	8.183	129 C6	150 O	8.218
129 C6	152 C	8.219	129 C6	38 CD2	8.265
129 C6	130 N	8.312	129 C6	151 O	8.336

Fig. 8R

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C6	130 O	8.337	129 C6	152 N	8.366
129 C6	150 C	8.619	129 C6	60 N	8.646
129 C6	301 OH2	8.647	129 C6	151 C	8.657
129 C6	150 CA	8.708	129 C6	127 CB	8.860
129 C6	130 C	8.881	129 C6	38 CG	8.985
129 C6	61 C	9.049	129 C6	152 O	9.088
129 C6	157 NH2	9.116	129 C6	150 N	9.137
129 C6	157 CA	9.146	129 C6	131 CB	9.173
129 C6	154 CG1	9.205	129 C6	128 CA	9.239
129 C6	130 CA	9.306	129 C6	131 N	9.377
129 C6	151 N	9.388	129 C6	131 CA	9.406
129 C6	157 CG	9.408	129 C6	128 N	9.432
129 C6	157 O	9.507	129 C6	127 OG	9.514
129 C6	157 CB	9.525	129 C6	127 C	9.547
129 C6	127 O	9.583	129 C6	61 O	9.616
129 C6	151 CA	9.685	129 C6	148 CE1	9.825
129 C6	157 CZ	9.884	129 C6	157 C	9.921
129 C6	157 NE	9.925	129 C6	127 CA	9.966
129 C6	38 CB	10.148	129 C6	154 CD1	10.257
129 C6	157 NH1	10.361	129 C6	149 C	10.363
129 C6	128 CB	10.409	129 C6	157 CD	10.439
129 C6	130 CB	10.498	129 C6	148 ND1	10.515
129 C6	148 NE2	10.556	129 C6	127 N	10.736
129 C6	148 O	10.806	129 C6	131 C	10.872
129 C6	149 CA	10.877	129 C6	151 CB	11.060
129 C6	128 CG2	11.113	129 C6	149 O	11.145
129 C6	132 N	11.157	129 C6	38 CA	11.160
129 C6	128 CG1	11.430	129 C6	27 O	11.460
129 C6	130 CG	11.594	129 C6	148 CG	11.646
129 C6	148 C	11.648	129 C6	148 CD2	11.659
129 C6	149 CB	11.748	129 C6	149 N	11.762
129 C6	38 N	11.818	129 C6	131 O	11.823
129 C7	152 SG	3.758	129 C7	61 ND1	3.773
129 C7	152 CB	3.840	129 C7	61 CE1	3.985
129 C7	60 OD1	4.142	129 C7	154 O	4.535
129 C7	61 CG	5.004	129 C7	60 CG	5.111
129 C7	155 CA	5.197	129 C7	61 NE2	5.222
129 C7	60 CA	5.334	129 C7	152 CA	5.348
129 C7	150 CB	5.402	129 C7	154 C	5.442
129 C7	60 C	5.606	129 C7	61 N	5.627
129 C7	61 CB	5.638	129 C7	156 CG	5.653
129 C7	155 N	5.750	129 C7	61 CD2	5.760
129 C7	60 OD2	5.814	129 C7	151 O	5.820
129 C7	60 CB	5.867	129 C7	156 N	5.871
129 C7	155 C	5.896	129 C7	152 N	5.972
129 C7	150 O	5.979	129 C7	151 C	6.159

Fig. 8S

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C7	152 C	6.184	129 C7	60 O	6.215
129 C7	150 C	6.280	129 C7	154 N	6.321
129 C7	60 N	6.334	129 C7	61 CA	6.339
129 C7	156 CD	6.404	129 C7	128 O	6.474
129 C7	150 CA	6.511	129 C7	128 C	6.512
129 C7	154 CA	6.632	129 C7	156 CB	6.650
129 C7	155 O	6.799	129 C7	300 OH2	6.850
129 C7	156 CA	6.927	129 C7	151 N	6.937
129 C7	156 NE	6.940	129 C7	152 O	7.077
129 C7	150 N	7.151	129 C7	151 CA	7.210
129 C7	131 OG	7.382	129 C7	127 CB	7.405
129 C7	128 CA	7.438	129 C7	130 N	7.442
129 C7	127 O	7.479	129 C7	154 CB	7.513
129 C7	127 C	7.664	129 C7	61 C	7.677
129 C7	128 N	7.706	129 C7	154 CG2	8.086
129 C7	130 O	8.161	129 C7	156 CZ	8.180
129 C7	127 CA	8.265	129 C7	301 OH2	8.274
129 C7	156 C	8.283	129 C7	127 OG	8.286
129 C7	130 C	8.377	129 C7	157 N	8.399
129 C7	149 C	8.431	129 C7	61 O	8.472
129 C7	130 CA	8.510	129 C7	151 CB	8.558
129 C7	148 CE1	8.655	129 C7	128 CB	8.706
129 C7	131 CB	8.766	129 C7	131 N	8.796
129 C7	154 CG1	8.811	129 C7	156 NH2	8.824
129 C7	127 N	8.941	129 C7	156 NH1	8.951
129 C7	131 CA	9.115	129 C7	149 O	9.117
129 C7	148 ND1	9.144	129 C7	149 CA	9.164
129 C7	156 O	9.340	129 C7	157 NH2	9.383
129 C7	128 CG1	9.531	129 C7	128 CG2	9.608
129 C7	148 O	9.622	129 C7	148 NE2	9.625
129 C7	157 O	9.718	129 C7	157 CA	9.769
129 C7	154 CD1	9.781	129 C7	38 CD2	9.806
129 C7	130 CB	9.829	129 C7	38 CD1	9.857
129 C7	151 CG	9.879	129 C7	151 CD1	9.915
129 C7	149 CB	9.979	129 C7	157 CB	9.980
129 C7	157 CG	10.096	129 C7	149 N	10.155
129 C7	148 C	10.282	129 C7	157 NE	10.285
129 C7	157 CZ	10.309	129 C7	157 C	10.332
129 C7	148 CG	10.394	129 C7	149 CG2	10.472
129 C7	38 CG	10.616	129 C7	131 C	10.653
129 C7	148 CD2	10.654	129 C7	151 CD2	10.973
129 C7	27 O	10.990	129 C7	157 CD	10.995
129 C7	130 CG	11.021	129 C7	157 NH1	11.032
129 C7	149 CG1	11.215	129 C7	132 N	11.226
129 C7	148 CB	11.373	129 C7	131 O	11.405
129 C7	148 CA	11.504	129 C7	27 CD1	11.505

Fig. 8T

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C7	130 CD1	11.547	129 C7	38 CB	11.568
129 C7	148 N	11.934	129 C7	27 C	11.970
129 C8	130 O	3.353	129 C8	157 NH2	4.087
129 C8	130 C	4.289	129 C8	61 CE1	4.327
129 C8	131 OG	4.632	129 C8	130 N	4.677
129 C8	61 NE2	4.786	129 C8	38 CD2	4.875
129 C8	131 CA	4.893	129 C8	156 NE	4.934
129 C8	131 N	4.978	129 C8	157 CZ	5.048
129 C8	301 OH2	5.112	129 C8	156 CB	5.132
129 C8	130 CA	5.146	129 C8	156 CG	5.226
129 C8	131 CB	5.362	129 C8	61 ND1	5.366
129 C8	157 NH1	5.431	129 C8	300 OH2	5.466
129 C8	156 NH2	5.542	129 C8	157 NE	5.573
129 C8	156 CD	5.675	129 C8	156 N	5.751
129 C8	156 CZ	5.763	129 C8	61 CD2	6.017
129 C8	130 CB	6.037	129 C8	156 CA	6.042
129 C8	131 C	6.132	129 C8	157 CG	6.151
129 C8	38 CG	6.159	129 C8	38 CD1	6.195
129 C8	132 N	6.220	129 C8	61 CG	6.327
129 C8	157 N	6.419	129 C8	157 CD	6.505
129 C8	156 C	6.607	129 C8	130 CG	6.818
129 C8	132 OG1	6.847	129 C8	155 C	6.863
129 C8	157 CB	6.864	129 C8	128 O	6.878
129 C8	38 CB	6.882	129 C8	155 CA	7.000
129 C8	156 NH1	7.064	129 C8	128 C	7.140
129 C8	131 O	7.182	129 C8	148 O	7.330
129 C8	157 CA	7.339	129 C8	38 CA	7.355
129 C8	150 CB	7.460	129 C8	156 O	7.461
129 C8	132 CA	7.565	129 C8	61 CB	7.697
129 C8	132 CB	7.710	129 C8	132 O	7.713
129 C8	130 CD2	7.719	129 C8	38 O	7.750
129 C8	132 CG2	7.755	129 C8	150 N	7.836
129 C8	130 CD1	7.846	129 C8	27 O	7.883
129 C8	152 SG	7.937	129 C8	155 O	7.956
129 C8	148 CE1	7.998	129 C8	150 O	8.064
129 C8	38 C	8.125	129 C8	132 C	8.220
129 C8	38 N	8.285	129 C8	150 CA	8.300
129 C8	148 NE2	8.340	129 C8	155 N	8.390
129 C8	154 O	8.397	129 C8	149 CA	8.426
129 C8	148 ND1	8.480	129 C8	148 C	8.492
129 C8	128 CA	8.582	129 C8	157 C	8.589
129 C8	150 C	8.659	129 C8	149 C	8.683
129 C8	157 O	8.691	129 C8	61 CA	8.833
129 C8	154 C	8.927	129 C8	152 CB	8.984
129 C8	61 N	9.019	129 C8	128 CB	9.023
129 C8	148 CD2	9.033	129 C8	149 N	9.047

Fig. 8U

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C8	27 C	9.057	129 C8	148 CG	9.123
129 C8	149 CB	9.254	129 C8	148 N	9.290
129 C8	128 N	9.342	129 C8	148 CA	9.567
129 C8	128 CG2	9.598	129 C8	27 CD1	9.621
129 C8	27 CA	9.622	129 C8	27 CG	9.684
129 C8	27 CB	9.689	129 C8	149 O	9.752
129 C8	60 C	9.755	129 C8	149 CG1	9.800
129 C8	151 N	9.903	129 C8	60 OD1	9.950
129 C8	148 CB	10.027	129 C8	60 CA	10.105
129 C8	61 C	10.126	129 C8	127 C	10.127
129 C8	128 CG1	10.136	129 C8	127 CB	10.201
129 C8	151 O	10.282	129 C8	61 O	10.292
129 C8	151 C	10.311	129 C8	152 N	10.328
129 C8	152 CA	10.350	129 C8	127 O	10.357
129 C8	60 O	10.362	129 C8	154 CA	10.464
129 C8	149 CG2	10.466	129 C8	151 CA	10.610
129 C8	60 CG	10.677	129 C8	60 N	10.827
129 C8	154 N	10.842	129 C8	127 CA	10.971
129 C8	27 N	11.011	129 C8	27 CD2	11.027
129 C8	152 C	11.125	129 C8	60 CB	11.140
129 C8	127 OG	11.141	129 C8	154 CG2	11.143
129 C8	60 OD2	11.249	129 C8	154 CB	11.309
129 C8	152 O	11.604	129 C9	130 O	3.586
129 C9	131 OG	3.727	129 C9	61 CE1	4.015
129 C9	131 CA	4.198	129 C9	61 NE2	4.279
129 C9	131 CB	4.392	129 C9	130 C	4.399
129 C9	131 N	4.688	129 C9	157 NH2	4.908
129 C9	61 ND1	4.928	129 C9	61 CD2	5.320
129 C9	130 N	5.410	129 C9	131 C	5.431
129 C9	132 N	5.453	129 C9	156 NE	5.538
129 C9	38 CD2	5.539	129 C9	130 CA	5.556
129 C9	61 CG	5.672	129 C9	156 NH2	5.756
129 C9	157 CZ	5.938	129 C9	157 NH1	6.119
129 C9	156 CZ	6.183	129 C9	156 CG	6.252
129 C9	132 OG1	6.318	129 C9	156 CB	6.362
129 C9	301 OH2	6.366	129 C9	156 CD	6.430
129 C9	130 CB	6.543	129 C9	131 O	6.555
129 C9	132 O	6.619	129 C9	157 NE	6.694
129 C9	132 CA	6.821	129 C9	300 OH2	6.937
129 C9	38 CG	6.970	129 C9	61 CB	6.976
129 C9	148 O	7.035	129 C9	130 CG	7.064
129 C9	148 CE1	7.121	129 C9	156 N	7.154
129 C9	132 CB	7.172	129 C9	38 CD1	7.197
129 C9	132 C	7.253	129 C9	148 NE2	7.297
129 C9	156 CA	7.412	129 C9	150 CB	7.431
129 C9	132 CG2	7.488	129 C9	157 CG	7.490

Fig. 8V

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C9	156 NH1	7.499	129 C9	157 CD	7.696
129 C9	148 ND1	7.769	129 C9	38 CB	7.773
129 C9	157 N	7.921	129 C9	130 CD1	7.943
129 C9	150 N	7.955	129 C9	156 C	8.040
129 C9	38 CA	8.042	129 C9	148 CD2	8.064
129 C9	130 CD2	8.087	129 C9	128 O	8.097
129 C9	148 C	8.166	129 C9	128 C	8.199
129 C9	61 CA	8.207	129 C9	155 C	8.232
129 C9	157 CB	8.311	129 C9	155 CA	8.314
129 C9	148 CG	8.347	129 C9	150 CA	8.402
129 C9	149 CA	8.462	129 C9	38 O	8.536
129 C9	150 O	8.594	129 C9	61 N	8.635
129 C9	148 N	8.657	129 C9	149 C	8.695
129 C9	152 SG	8.791	129 C9	38 N	8.821
129 C9	157 CA	8.824	129 C9	156 O	8.834
129 C9	149 N	8.864	129 C9	38 C	8.884
129 C9	150 C	9.002	129 C9	148 CA	9.056
129 C9	27 O	9.059	129 C9	155 O	9.314
129 C9	61 C	9.367	129 C9	61 O	9.373
129 C9	148 CB	9.387	129 C9	154 O	9.437
129 C9	60 C	9.440	129 C9	149 CB	9.486
129 C9	128 CA	9.576	129 C9	152 CB	9.617
129 C9	155 N	9.655	129 C9	149 O	9.666
129 C9	60 O	9.935	129 C9	149 CG1	9.989
129 C9	128 CB	9.993	129 C9	60 CA	10.021
129 C9	154 C	10.077	129 C9	60 OD1	10.106
129 C9	157 C	10.106	129 C9	27 C	10.195
129 C9	157 O	10.223	129 C9	151 N	10.236
129 C9	27 CD1	10.388	129 C9	27 CG	10.403
129 C9	128 N	10.450	129 C9	27 CB	10.557
129 C9	151 O	10.624	129 C9	27 CA	10.663
129 C9	60 CG	10.678	129 C9	128 CG2	10.703
129 C9	149 CG2	10.711	129 C9	60 N	10.792
129 C9	151 C	10.804	129 C9	128 CG1	10.976
129 C9	152 N	10.976	129 C9	152 CA	10.995
129 C9	60 CB	11.095	129 C9	151 CA	11.101
129 C9	60 OD2	11.148	129 C9	127 C	11.182
129 C9	127 O	11.281	129 C9	127 CB	11.407
129 C9	154 CA	11.603	129 C9	27 CD2	11.656
129 C9	154 N	11.860	129 C9	152 C	11.913
129 C10	38 CD2	3.359	129 C10	157 NH2	3.705
129 C10	130 O	3.997	129 C10	156 NE	4.242
129 C10	157 CZ	4.340	129 C10	156 CB	4.479
129 C10	157 NH1	4.489	129 C10	156 NH2	4.536
129 C10	38 CG	4.654	129 C10	38 CD1	4.809
129 C10	157 NE	4.863	129 C10	156 CZ	4.878

Fig. 8W

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C10 156 CG		4.880	129 C10 130 C		5.125
129 C10 157 CG		5.172	129 C10 156 CD		5.186
129 C10 301 OH2		5.236	129 C10 38 CB		5.403
129 C10 156 CA		5.510	129 C10 130 N		5.529
129 C10 157 CD		5.570	129 C10 300 OH2		5.577
129 C10 156 N		5.581	129 C10 157 N		5.755
129 C10 131 CA		5.762	129 C10 61 CE1		5.817
129 C10 156 C		5.851	129 C10 38 CA		5.897
129 C10 131 OG		5.920	129 C10 131 N		5.930
129 C10 130 CA		5.964	129 C10 157 CB		6.108
129 C10 156 NH1		6.174	129 C10 61 NE2		6.296
129 C10 131 CB		6.439	129 C10 38 O		6.518
129 C10 156 O		6.529	129 C10 130 CB		6.549
129 C10 157 CA		6.554	129 C10 132 N		6.589
129 C10 132 OG1		6.590	129 C10 131 C		6.763
129 C10 38 C		6.766	129 C10 61 ND1		6.793
129 C10 38 N		6.796	129 C10 155 C		6.836
129 C10 130 CG		7.249	129 C10 155 CA		7.277
129 C10 61 CD2		7.505	129 C10 128 O		7.520
129 C10 132 CB		7.634	129 C10 132 CG2		7.668
129 C10 132 CA		7.776	129 C10 61 CG		7.783
129 C10 27 O		7.802	129 C10 155 O		7.807
129 C10 131 O		7.860	129 C10 132 O		7.889
129 C10 130 CD2		7.892	129 C10 157 C		7.943
129 C10 128 C		7.972	129 C10 157 O		8.232
129 C10 132 C		8.424	129 C10 130 CD1		8.463
129 C10 148 O		8.481	129 C10 155 N		8.705
129 C10 154 O		8.824	129 C10 152 SG		8.902
129 C10 150 CB		8.943	129 C10 27 C		9.013
129 C10 61 CB		9.111	129 C10 150 N		9.224
129 C10 154 C		9.305	129 C10 150 O		9.329
129 C10 148 CE1		9.399	129 C10 128 CA		9.451
129 C10 148 NE2		9.643	129 C10 149 CA		9.681
129 C10 148 C		9.688	129 C10 150 CA		9.735
129 C10 27 CA		9.799	129 C10 128 CB		9.831
129 C10 148 ND1		9.879	129 C10 27 CB		9.922
129 C10 150 C		10.013	129 C10 149 C		10.047
129 C10 152 CB		10.063	129 C10 128 N		10.092
129 C10 27 CG		10.130	129 C10 128 CG2		10.210
129 C10 27 CD1		10.219	129 C10 148 CD2		10.283
129 C10 149 N		10.297	129 C10 61 CA		10.299
129 C10 148 N		10.336	129 C10 149 CB		10.401
129 C10 148 CG		10.433	129 C10 61 N		10.484
129 C10 148 CA		10.731	129 C10 127 CB		10.784
129 C10 149 CG1		10.836	129 C10 154 CA		10.853
129 C10 127 C		10.939	129 C10 128 CG1		11.046

Fig. 8X

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C10	60 OD1	11.098	129 C10	149 O	11.152
129 C10	27 N	11.156	129 C10	60 C	11.169
129 C10	154 CG2	11.206	129 C10	151 N	11.255
129 C10	148 CB	11.295	129 C10	127 O	11.306
129 C10	154 N	11.408	129 C10	152 CA	11.439
129 C10	27 CD2	11.469	129 C10	152 N	11.471
129 C10	60 CA	11.487	129 C10	151 C	11.565
129 C10	61 C	11.566	129 C10	154 CB	11.567
129 C10	127 OG	11.597	129 C10	151 O	11.597
129 C10	127 CA	11.653	129 C10	149 CG2	11.662
129 C10	61 O	11.698	129 C10	60 O	11.736
129 C10	151 CA	11.878	129 C10	60 CG	11.886

Fig. 9A

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 N	128 C	1.313	129 N	128 O	2.229
129 N	128 CA	2.384	129 N	128 CB	3.053
129 N	130 N	3.368	129 N	128 N	3.513
129 N	128 CG2	3.559	129 N	321 OH2	3.837
129 N	152 SG	4.323	129 N	128 CG1	4.378
129 N	130 CA	4.579	129 N	152 N	5.419
129 N	130 CB	5.512	129 N	61 NE2	5.531
129 N	130 C	5.542	129 N	27 CD1	5.545
129 N	152 CB	5.593	129 N	61 CE1	5.741
129 N	130 O	5.971	129 N	152 CA	6.168
129 N	131 N	6.179	129 N	27 O	6.333
129 N	156 N	6.399	129 N	61 CD2	6.575
129 N	27 CA	6.610	129 N	148 O	6.652
129 N	27 CG	6.673	129 N	61 ND1	6.819
129 N	152 C	6.917	129 N	27 CB	6.923
129 N	27 C	6.934	129 N	152 O	6.936
129 N	130 CG	7.019	129 N	148 C	7.098
129 N	157 NH2	7.106	129 N	131 OG	7.208
129 N	157 N	7.293	129 N	61 CG	7.293
129 N	131 CA	7.356	129 N	148 ND1	7.428
129 N	130 CD1	7.482	129 N	157 NE	7.533
129 N	148 CE1	7.567	129 N	157 CZ	7.625
129 N	156 CA	7.631	129 N	157 CB	7.633
129 N	27 N	7.688	129 N	157 O	7.730
129 N	130 CD2	7.812	129 N	131 CB	7.817
129 N	61 N	7.918	129 N	156 CB	7.929
129 N	27 CD2	7.952	129 N	156 C	8.043
129 N	157 CA	8.045	129 N	157 CG	8.099

Fig. 9B

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 N	157 C	8.370	129 N	148 CG	8.456
129 N	131 C	8.489	129 N	157 CD	8.490
129 N	61 CB	8.557	129 N	61 CA	8.571
129 N	157 NH1	8.577	129 N	148 CA	8.599
129 N	148 NE2	8.600	129 N	131 O	8.638
129 N	148 CB	8.960	129 N	148 CD2	9.109
129 N	156 O	9.204	129 N	148 N	9.209
129 N	156 CG	9.248	129 N	156 CD	9.593
129 N	156 NE	9.904	129 N	61 C	10.040
129 N	61 O	10.738	129 N	156 CZ	11.017
129 N	156 NH1	11.432	129 N	156 NH2	11.852
129 CA	128 C	2.383	129 CA	130 N	2.442
129 CA	128 O	2.714	129 CA	321 OH2	3.213
129 CA	128 CA	3.727	129 CA	130 CA	3.795
129 CA	128 CB	4.338	129 CA	130 C	4.521
129 CA	128 CG2	4.540	129 CA	128 N	4.679
129 CA	152 SG	4.741	129 CA	130 O	4.764
129 CA	61 NE2	4.812	129 CA	130 CB	4.821
129 CA	61 CE1	4.969	129 CA	131 N	5.268
129 CA	156 N	5.726	129 CA	128 CG1	5.727
129 CA	27 CD1	5.933	129 CA	27 O	5.957
129 CA	157 NH2	5.968	129 CA	61 CD2	6.029
129 CA	152 CB	6.080	129 CA	61 ND1	6.182
129 CA	131 OG	6.238	129 CA	148 O	6.293
129 CA	130 CG	6.321	129 CA	131 CA	6.326
129 CA	152 N	6.394	129 CA	157 CZ	6.452
129 CA	157 NE	6.489	129 CA	157 N	6.552
129 CA	27 CA	6.693	129 CA	27 C	6.769

Fig. 9C

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CA	61 CG	6.769	129 CA	156 CA	6.812
129 CA	27 CG	6.812	129 CA	157 CB	6.850
129 CA	131 CB	6.879	129 CA	27 CB	6.898
129 CA	156 CB	6.912	129 CA	152 CA	6.934
129 CA	148 C	6.936	129 CA	130 CD1	6.964
129 CA	157 CG	7.101	129 CA	148 CE1	7.184
129 CA	130 CD2	7.187	129 CA	156 C	7.213
129 CA	148 ND1	7.221	129 CA	157 NH1	7.310
129 CA	157 CA	7.340	129 CA	157 O	7.435
129 CA	157 CD	7.469	129 CA	131 C	7.507
129 CA	152 C	7.713	129 CA	131 O	7.809
129 CA	152 O	7.881	129 CA	157 C	7.905
129 CA	27 N	7.931	129 CA	61 N	7.937
129 CA	148 NE2	8.073	129 CA	61 CB	8.151
129 CA	148 CG	8.183	129 CA	27 CD2	8.203
129 CA	156 CG	8.254	129 CA	156 O	8.317
129 CA	61 CA	8.397	129 CA	148 CA	8.406
129 CA	156 CD	8.508	129 CA	148 CD2	8.653
129 CA	156 NE	8.688	129 CA	148 N	8.803
129 CA	148 CB	8.819	129 CA	156 CZ	9.760
129 CA	61 C	9.887	129 CA	156 NH1	10.103
129 CA	61 O	10.466	129 CA	156 NH2	10.648
129 CB	128 C	3.238	129 CB	321 OH2	3.477
129 CB	128 O	3.494	129 CB	130 N	3.511
129 CB	61 NE2	3.522	129 CB	152 SG	3.945
129 CB	61 CE1	3.969	129 CB	128 CA	4.473
129 CB	61 CD2	4.694	129 CB	130 CA	4.740
129 CB	130 C	5.074	129 CB	152 CB	5.139

Fig. 9D

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CB	130 O	5.184	129 CB	61 ND1	5.204
129 CB	128 N	5.255	129 CB	156 N	5.317
129 CB	128 CB	5.405	129 CB	61 CG	5.592
129 CB	131 N	5.629	129 CB	128 CG2	5.814
129 CB	131 OG	5.835	129 CB	152 N	5.936
129 CB	130 CB	5.951	129 CB	152 CA	6.226
129 CB	156 CB	6.348	129 CB	156 CA	6.431
129 CB	131 CA	6.449	129 CB	128 CG1	6.683
129 CB	157 NH2	6.716	129 CB	157 N	6.727
129 CB	131 CB	6.748	129 CB	148 CE1	6.763
129 CB	148 O	6.845	129 CB	61 N	6.897
129 CB	61 CB	6.989	129 CB	148 ND1	7.051
129 CB	157 CZ	7.089	129 CB	152 C	7.103
129 CB	156 C	7.129	129 CB	157 NE	7.241
129 CB	27 O	7.275	129 CB	130 CG	7.368
129 CB	61 CA	7.372	129 CB	27 CD1	7.416
129 CB	148 C	7.428	129 CB	157 CB	7.458
129 CB	152 O	7.494	129 CB	156 CG	7.533
129 CB	157 CG	7.575	129 CB	156 CD	7.617
129 CB	148 NE2	7.651	129 CB	157 NH1	7.733
129 CB	157 CA	7.743	129 CB	131 C	7.804
129 CB	156 NE	7.910	129 CB	157 O	7.920
129 CB	130 CD1	7.987	129 CB	157 CD	8.107
129 CB	148 CG	8.133	129 CB	27 C	8.160
129 CB	27 CA	8.176	129 CB	156 O	8.230
129 CB	131 O	8.273	129 CB	27 CG	8.293
129 CB	130 CD2	8.359	129 CB	27 CB	8.382
129 CB	157 C	8.405	129 CB	148 CD2	8.453

Fig. 9E

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 CB	148 CA	8.800	129 CB	61 C	8.881
129 CB	156 CZ	8.941	129 CB	148 CB	8.990
129 CB	148 N	9.160	129 CB	156 NH1	9.403
129 CB	27 N	9.413	129 CB	61 O	9.484
129 CB	27 CD2	9.684	129 CB	156 NH2	9.697
129 OG	61 NE2	3.211	129 OG	321 OH2	3.564
129 OG	130 N	3.619	129 OG	61 CE1	3.630
129 OG	128 C	4.434	129 OG	128 O	4.438
129 OG	61 CD2	4.510	129 OG	130 O	4.520
129 OG	130 C	4.700	129 OG	130 CA	4.737
129 OG	152 SG	4.869	129 OG	156 N	4.951
129 OG	61 ND1	4.957	129 OG	131 OG	5.240
129 OG	131 N	5.294	129 OG	61 CG	5.418
129 OG	156 CB	5.456	129 OG	128 CA	5.777
129 OG	156 CA	5.824	129 OG	131 CA	5.863
129 OG	130 CB	5.918	129 OG	152 CB	6.023
129 OG	157 NH2	6.062	129 OG	131 CB	6.210
129 OG	157 N	6.306	129 OG	157 CZ	6.328
129 OG	128 N	6.479	129 OG	156 CD	6.538
129 OG	156 C	6.538	129 OG	156 CG	6.606
129 OG	157 NE	6.627	129 OG	128 CB	6.647
129 OG	156 NE	6.684	129 OG	157 NH1	6.781
129 OG	148 CE1	6.821	129 OG	128 CG2	6.880
129 OG	61 CB	6.892	129 OG	157 CG	6.909
129 OG	148 O	7.020	129 OG	157 CB	7.045
129 OG	152 N	7.152	129 OG	130 CG	7.220
129 OG	131 C	7.241	129 OG	152 CA	7.271
129 OG	61 N	7.286	129 OG	148 ND1	7.301

Fig. 9F

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 OG	157 CA	7.352	129 OG	27 O	7.382
129 OG	157 CD	7.440	129 OG	148 NE2	7.511
129 OG	156 O	7.533	129 OG	61 CA	7.542
129 OG	156 CZ	7.656	129 OG	148 C	7.748
129 OG	131 O	7.892	129 OG	157 O	7.929
129 OG	128 CG1	7.981	129 OG	130 CD1	7.982
129 OG	156 NH1	8.055	129 OG	152 C	8.115
129 OG	27 CD1	8.126	129 OG	130 CD2	8.232
129 OG	157 C	8.236	129 OG	148 CG	8.282
129 OG	148 CD2	8.389	129 OG	27 C	8.403
129 OG	156 NH2	8.453	129 OG	152 O	8.599
129 OG	27 CA	8.623	129 OG	27 CB	8.757
129 OG	27 CG	8.806	129 OG	61 C	9.020
129 OG	148 CA	9.033	129 OG	148 N	9.176
129 OG	148 CB	9.252	129 OG	61 O	9.484
129 OG	27 N	9.941	129 OG	27 CD2	10.246
129 C	130 N	1.326	129 C	130 CA	2.411
129 C	130 C	3.213	129 C	128 C	3.490
129 C	130 CB	3.635	129 C	130 O	3.724
129 C	131 N	3.885	129 C	128 O	3.993
129 C	321 OH2	4.454	129 C	128 CA	4.611
129 C	61 CE1	4.678	129 C	128 CB	4.808
129 C	148 O	4.818	129 C	61 NE2	4.933
129 C	128 CG2	4.974	129 C	130 CG	5.058
129 C	131 CA	5.072	129 C	131 OG	5.277
129 C	27 CD1	5.335	129 C	157 NH2	5.362
129 C	148 C	5.539	129 C	130 CD1	5.558
129 C	131 CB	5.695	129 C	128 N	5.785

Fig. 9G

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 C	61 ND1	5.801	129 C	27 O	5.865
129 C	152 SG	6.060	129 C	27 CG	6.064
129 C	130 CD2	6.097	129 C	157 CZ	6.127
129 C	131 C	6.168	129 C	128 CG1	6.177
129 C	148 ND1	6.186	129 C	61 CD2	6.194
129 C	148 CE1	6.273	129 C	27 CB	6.327
129 C	131 O	6.367	129 C	157 NE	6.390
129 C	27 CA	6.461	129 C	61 CG	6.655
129 C	27 C	6.660	129 C	156 N	6.982
129 C	148 CG	6.997	129 C	157 NH1	7.004
129 C	148 CA	7.009	129 C	148 NE2	7.079
129 C	152 CB	7.217	129 C	148 N	7.349
129 C	152 N	7.356	129 C	157 CB	7.421
129 C	27 CD2	7.449	129 C	157 CG	7.493
129 C	148 CD2	7.493	129 C	157 N	7.522
129 C	148 CB	7.544	129 C	157 CD	7.576
129 C	27 N	7.785	129 C	156 CB	7.850
129 C	156 CA	7.920	129 C	61 N	7.951
129 C	61 CB	8.011	129 C	152 CA	8.029
129 C	157 CA	8.158	129 C	156 C	8.206
129 C	61 CA	8.206	129 C	157 O	8.497
129 C	157 C	8.829	129 C	152 C	8.946
129 C	152 O	9.119	129 C	156 CG	9.199
129 C	156 O	9.221	129 C	156 NE	9.287
129 C	156 CD	9.312	129 C	61 C	9.634
129 C	61 O	10.088	129 C	156 CZ	10.241
129 C	156 NH1	10.408	129 C	156 NH2	11.188
129 O	130 N	2.224	129 O	130 CA	2.723

Fig. 9H

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O	130 C	3.426	129 O	131 N	3.695
129 O	128 C	3.990	129 O	148 O	4.045
129 O	130 CB	4.093	129 O	130 O	4.206
129 O	61 CE1	4.301	129 O	148 C	4.586
129 O	61 NE2	4.732	129 O	128 O	4.758
129 O	128 CA	4.824	129 O	131 OG	4.902
129 O	131 CA	4.923	129 O	128 CB	4.938
129 O	148 ND1	5.094	129 O	61 ND1	5.235
129 O	131 CB	5.297	129 O	148 CE1	5.306
129 O	130 CG	5.351	129 O	128 CG2	5.375
129 O	130 CD1	5.522	129 O	321 OH2	5.529
129 O	27 CD1	5.540	129 O	61 CD2	5.862
129 O	148 CG	5.954	129 O	131 C	6.037
129 O	148 CA	6.055	129 O	131 O	6.122
129 O	61 CG	6.130	129 O	128 N	6.135
129 O	128 CG1	6.169	129 O	148 NE2	6.209
129 O	157 NH2	6.258	129 O	152 SG	6.273
129 O	27 CG	6.346	129 O	148 CB	6.478
129 O	130 CD2	6.537	129 O	148 N	6.546
129 O	148 CD2	6.565	129 O	27 O	6.839
129 O	27 CB	6.870	129 O	152 N	7.121
129 O	157 CZ	7.139	129 O	27 CA	7.146
129 O	61 N	7.172	129 O	152 CB	7.181
129 O	61 CB	7.379	129 O	61 CA	7.403
129 O	157 NE	7.496	129 O	27 C	7.534
129 O	27 CD2	7.629	129 O	152 CA	7.902
129 O	157 NH1	7.972	129 O	156 N	7.976
129 O	27 N	8.418	129 O	157 CB	8.636

Fig. 9I

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
129 O	157 CG	8.689	129 O	157 N	8.697
129 O	157 CD	8.727	129 O	61 C	8.783
129 O	156 CB	8.843	129 O	152 C	8.964
129 O	156 CA	8.968	129 O	152 O	9.169
129 O	61 O	9.242	129 O	156 C	9.344
129 O	157 CA	9.365	129 O	157 O	9.632
129 O	157 C	10.010	129 O	156 NE	10.127
129 O	156 CG	10.130	129 O	156 CD	10.137
129 O	156 O	10.370	129 O	156 CZ	11.020
129 O	156 NH1	11.186	129 O	156 NH2	11.901

Fig. 10A.

<u>Atom 1</u>	<u>Atom 2</u>	<u>Dist.</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Dist.</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Dist.</u>
61CA	148CE1	4.683	61CB	148CE1	4.657	61CG	148CE1	4.271
61CG	129OG	4.982	61CD2	129OG	4.142	61CD2	129CB	4.339
61CD2	148CE1	4.601	61CD2	129O	4.620	61ND1	148CE1	4.255
61ND1	129OG	4.534	61ND1	131CB	4.746	61ND1	148NE2	4.920
61CE1	129OG	3.291	61CE1	129CB	4.134	61CE1	129O	4.249
61CE1	131CB	4.357	61CE1	148CE1	4.581	61CE1	129C	4.708
61CE1	131CA	4.974	61CE1	131N	4.990	61NE2	129OG	2.922
61NE2	129CB	3.336	61NE2	129O	3.621	61NE2	129C	4.171
61NE2	129CA	4.389	61NE2	148CE1	4.781	129N	152SG	4.570
129CA	61NE2	4.389	129CA	152SG	4.909	129CB	61NE2	3.336
129CB	152SG	4.005	129CB	61CE1	4.134	129CB	61CD2	4.339
129OG	61NE2	2.922	129OG	61CE1	3.291	129OG	61CD2	4.142
129OG	61ND1	4.534	129OG	156CG	4.962	129OG	152SG	4.970
129OG	61CG	4.982	129C	131N	3.961	129C	61NE2	4.171
129C	148O	4.545	129C	61CE1	4.708	129O	61NE2	3.621
129O	131N	3.740	129O	148O	3.795	129O	61CE1	4.249
129O	148C	4.547	129O	61CD2	4.620	129O	131CA	4.908
131N	148O	2.713	131N	129O	3.740	131N	148C	3.953
131N	129C	3.961	131N	148N	4.427	131N	148CA	4.842
131N	157NH2	4.894	131N	61CE1	4.990	131CA	148O	3.706
131CA	148N	4.689	131CA	148C	4.843	131CA	129O	4.908
131CA	61CE1	4.974	131CB	148NE2	3.715	131CB	148O	3.761
131CB	148CD2	3.987	131CB	148CE1	3.997	131CB	61CE1	4.357
131CB	148ND1	4.391	131CB	148CG	4.407	131CB	148N	4.420
131CB	148C	4.685	131CB	61ND1	4.746	131C	148O	4.240
131C	148N	4.409	131O	148N	3.456	131O	148O	3.765
131O	148C	4.599	131O	148CA	4.633	148N	131O	3.456
148N	131C	4.409	148N	131CB	4.420	148N	131N	4.427
148N	131CA	4.689	148CA	131O	4.633	148CA	131N	4.842
148CG	131CB	4.407	148CD2	131CB	3.987	148ND1	131CB	4.391
148CE1	131CB	3.997	148CE1	61ND1	4.255	148CE1	61CG	4.271

Fig. 10B

<u>Atom 1</u>	<u>Atom 2</u>	<u>Dist.</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Dist.</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Dist.</u>
148CE1	61CE1	4.581	148CE1	61CD2	4.601	148CE1	61CB	4.657
148CE1	61CA	4.683	148CE1	61NE2	4.781	148NE2	131CB	3.715
148NE2	61ND1	4.920	148C	131N	3.953	148C	129O	4.547
148C	131O	4.599	148C	131CB	4.685	148C	131CA	4.843
148O	131N	2.713	148O	131CA	3.706	148O	131CB	3.761
148O	131O	3.765	148O	129O	3.795	148O	131C	4.240
148O	129C	4.545	152SG	129CB	4.005	152SG	129N	4.570
152SG	129CA	4.909	152SG	129OG	4.970	156N	157N	2.799
156N	157CA	4.227	156N	157O	4.299	156N	157C	4.735
156N	157CB	4.979	156CA	157N	2.426	156CA	157CA	3.792
156CA	157O	4.393	156CA	157C	4.516	156CA	157CB	4.758
156CB	157N	3.389	156CB	157CA	4.669	156CG	157N	4.416
156CG	129OG	4.962	156C	157N	1.316	156C	157CA	2.399
156C	157C	3.245	156C	157O	3.454	156C	157CB	3.557
156C	157CG	3.912	156O	157N	2.214	156O	157CA	2.690
156O	157C	3.474	156O	157O	3.931	156O	157CB	3.972
156O	157CG	4.193	157N	156C	1.316	157N	156O	2.214
157N	156CA	2.426	157N	156N	2.799	157N	156CB	3.389
157N	156CG	4.416	157CA	156C	2.399	157CA	156O	2.690
157CA	156CA	3.792	157CA	156N	4.227	157CA	156CB	4.669
157CB	156C	3.557	157CB	156O	3.972	157CB	156CA	4.758
157CB	156N	4.979	157CG	156C	3.912	157CG	156O	4.193
157NH2	131N	4.894	157C	156C	3.245	157C	156O	3.474
157C	156CA	4.516	157C	156N	4.735	157O	156C	3.454
157O	156O	3.931	157O	156N	4.299	157O	156CA	4.393

Fig. 11A

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 C	129 N	128 O	27.78	128 C	129 N	128 CA	35.07
128 C	129 N	128 CB	53.60	128 C	129 N	130 N	131.02
128 C	129 N	128 N	20.09	128 C	129 N	128 CG1	67.65
128 C	129 N	128 CG2	43.80	128 C	129 N	300 OH2	65.57
128 C	129 N	301 OH2	90.41	128 C	129 N	130 CA	137.76
128 C	129 N	152 SG	68.42	128 C	129 N	130 CB	124.22
128 C	129 N	27 CD1	92.40	128 C	129 N	130 C	143.31
128 C	129 N	61 CE1	138.31	128 C	129 N	152 N	72.55
128 C	129 N	61 NE2	151.25	128 C	129 N	130 O	135.18
128 C	129 N	152 CB	77.98	128 O	129 N	128 CA	62.79
128 O	129 N	128 CB	75.52	128 O	129 N	130 N	109.67
128 O	129 N	128 N	47.34	128 O	129 N	128 CG1	92.42
128 O	129 N	128 CG2	60.40	128 O	129 N	300 OH2	38.19
128 O	129 N	301 OH2	68.39	128 O	129 N	130 CA	119.47
128 O	129 N	152 SG	69.72	128 O	129 N	130 CB	109.53
128 O	129 N	27 CD1	98.81	128 O	129 N	130 C	119.76
128 O	129 N	61 CE1	120.22	128 O	129 N	152 N	87.80
128 O	129 N	61 NE2	132.37	128 O	129 N	130 O	109.59
128 O	129 N	152 CB	82.37	128 CA	129 N	128 CB	31.92
128 CA	129 N	130 N	144.31	128 CA	129 N	128 N	17.71
128 CA	129 N	128 CG1	37.17	128 CA	129 N	128 CG2	37.17
128 CA	129 N	300 OH2	99.90	128 CA	129 N	301 OH2	116.05
128 CA	129 N	130 CA	141.26	128 CA	129 N	152 SG	76.56
128 CA	129 N	130 CB	128.79	128 CA	129 N	27 CD1	81.21
128 CA	129 N	130 C	154.23	128 CA	129 N	61 CE1	146.19
128 CA	129 N	152 N	60.89	128 CA	129 N	61 NE2	149.59
128 CA	129 N	130 O	157.70	128 CA	129 N	152 CB	79.10
128 CB	129 N	130 N	113.66	128 CB	129 N	128 N	45.76
128 CB	129 N	128 CG1	18.75	128 CB	129 N	128 CG2	18.18

Fig. 11B

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 CB	129 N	300 OH2	102.48	128 CB	129 N	301 OH2	98.82
128 CB	129 N	130 CA	109.37	128 CB	129 N	152 SG	108.47
128 CB	129 N	130 CB	97.50	128 CB	129 N	27 CD1	49.33
128 CB	129 N	130 C	122.36	128 CB	129 N	61 CE1	162.96
128 CB	129 N	152 N	89.08	128 CB	129 N	61 NE2	152.10
128 CB	129 N	130 O	127.99	128 CB	129 N	152 CB	110.07
130 N	129 N	128 N	147.37	130 N	129 N	128 CG1	115.80
130 N	129 N	128 CG2	107.47	130 N	129 N	300 OH2	74.30
130 N	129 N	301 OH2	41.52	130 N	129 N	130 CA	11.22
130 N	129 N	152 SG	136.22	130 N	129 N	130 CB	16.40
130 N	129 N	27 CD1	65.01	130 N	129 N	130 C	12.93
130 N	129 N	61 CE1	69.16	130 N	129 N	152 N	153.81
130 N	129 N	61 NE2	62.79	130 N	129 N	130 O	14.40
130 N	129 N	152 CB	136.24	128 N	129 N	128 CG1	54.48
128 N	129 N	128 CG2	44.02	128 N	129 N	300 OH2	85.46
128 N	129 N	301 OH2	109.26	128 N	129 N	130 CA	150.10
128 N	129 N	152 SG	65.04	128 N	129 N	130 CB	135.82
128 N	129 N	27 CD1	93.01	128 N	129 N	130 C	160.29
128 N	129 N	61 CE1	139.12	128 N	129 N	152 N	58.50
128 N	129 N	61 NE2	148.56	128 N	129 N	130 O	154.73
128 N	129 N	152 CB	70.88	128 CG1	129 N	128 CG2	36.88
128 CG1	129 N	300 OH2	121.22	128 CG1	129 N	301 OH2	113.17
128 CG1	129 N	130 CA	108.19	128 CG1	129 N	152 SG	107.90
128 CG1	129 N	130 CB	99.65	128 CG1	129 N	27 CD1	52.13
128 CG1	129 N	130 C	120.44	128 CG1	129 N	61 CE1	144.24
128 CG1	129 N	152 N	81.54	128 CG1	129 N	61 NE2	134.44
128 CG1	129 N	130 O	129.62	128 CG1	129 N	152 CB	105.10
128 CG2	129 N	300 OH2	84.35	128 CG2	129 N	301 OH2	83.51
128 CG2	129 N	130 CA	106.72	128 CG2	129 N	152 SG	108.86

Fig. 11C

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 CG2	129 N	130 CB	92.93	128 CG2	129 N	27 CD1	49.78
128 CG2	129 N	130 C	118.86	128 CG2	129 N	61 CE1	176.63
128 CG2	129 N	152 N	98.06	128 CG2	129 N	61 NE2	164.94
128 CG2	129 N	130 O	120.53	128 CG2	129 N	152 CB	114.63
300 OH2	129 N	301 OH2	37.04	300 OH2	129 N	130 CA	85.23
300 OH2	129 N	152 SG	85.78	300 OH2	129 N	130 CB	79.65
300 OH2	129 N	27 CD1	96.74	300 OH2	129 N	130 C	82.52
300 OH2	129 N	61 CE1	94.48	300 OH2	129 N	152 N	114.85
300 OH2	129 N	61 NE2	102.75	300 OH2	129 N	130 O	71.73
300 OH2	129 N	152 CB	97.96	301 OH2	129 N	130 CA	51.10
301 OH2	129 N	152 SG	121.22	301 OH2	129 N	130 CB	43.03
301 OH2	129 N	27 CD1	67.96	301 OH2	129 N	130 C	52.98
301 OH2	129 N	61 CE1	93.65	301 OH2	129 N	152 N	151.80
301 OH2	129 N	61 NE2	94.17	301 OH2	129 N	130 O	45.53
301 OH2	129 N	152 CB	131.91	130 CA	129 N	152 SG	142.15
130 CA	129 N	130 CB	14.34	130 CA	129 N	27 CD1	60.05
130 CA	129 N	130 C	12.99	130 CA	129 N	61 CE1	70.00
130 CA	129 N	152 N	149.69	130 CA	129 N	61 NE2	61.34
130 CA	129 N	130 O	21.72	130 CA	129 N	152 CB	138.64
152 SG	129 N	130 CB	152.45	152 SG	129 N	27 CD1	157.72
152 SG	129 N	130 C	129.15	152 SG	129 N	61 CE1	74.16
152 SG	129 N	152 N	31.77	152 SG	129 N	61 NE2	85.11
152 SG	129 N	130 O	122.05	152 SG	129 N	152 CB	13.04
130 CB	129 N	27 CD1	48.62	130 CB	129 N	130 C	25.95
130 CB	129 N	61 CE1	83.74	130 CB	129 N	152 N	162.50
130 CB	129 N	61 NE2	75.60	130 CB	129 N	130 O	30.77
130 CB	129 N	152 CB	152.09	27 CD1	129 N	130 C	73.04
27 CD1	129 N	61 CE1	127.40	27 CD1	129 N	152 N	133.24
27 CD1	129 N	61 NE2	115.61	27 CD1	129 N	130 O	79.39

Fig. 11D

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
27 CD1	129 N	152 CB	157.15	130 C	129 N	61 CE1	57.80
130 C	129 N	152 N	141.13	130 C	129 N	61 NE2	50.34
130 C	129 N	130 O	11.69	130 C	129 N	152 CB	126.24
61 CE1	129 N	152 N	85.31	61 CE1	129 N	61 NE2	13.10
61 CE1	129 N	130 O	56.11	61 CE1	129 N	152 CB	68.65
152 N	129 N	61 NE2	91.02	152 N	129 N	130 O	141.41
152 N	129 N	152 CB	24.01	61 NE2	129 N	130 O	51.58
61 NE2	129 N	152 CB	77.90	130 O	129 N	152 CB	121.94
128 C	129 CA	130 N	125.69	128 C	129 CA	128 O	27.01
128 C	129 CA	301 OH2	98.02	128 C	129 CA	300 OH2	77.47
128 C	129 CA	128 CA	13.00	128 C	129 CA	130 CA	128.11
128 C	129 CA	128 CB	28.37	128 C	129 CA	130 C	146.45
128 C	129 CA	130 O	152.69	128 C	129 CA	128 N	5.31
128 C	129 CA	130 CB	117.06	128 C	129 CA	61 CE1	136.63
128 C	129 CA	152 SG	60.33	128 C	129 CA	128 CG2	28.36
128 C	129 CA	61 NE2	140.27	128 C	129 CA	128 CG1	36.20
128 C	129 CA	131 N	147.20	128 C	129 CA	157 NH2	130.71
128 C	129 CA	156 N	89.11	128 C	129 CA	27 O	81.50
128 C	129 CA	61 ND1	128.82	128 C	129 CA	131 OG	157.02
128 C	129 CA	27 CD1	70.88	130 N	129 CA	128 O	125.80
130 N	129 CA	301 OH2	53.64	130 N	129 CA	300 OH2	97.55
130 N	129 CA	128 CA	121.50	130 N	129 CA	130 CA	9.21
130 N	129 CA	128 CB	100.10	130 N	129 CA	130 C	21.73
130 N	129 CA	130 O	29.22	130 N	129 CA	128 N	131.00
130 N	129 CA	130 CB	8.71	130 N	129 CA	61 CE1	92.68
130 N	129 CA	152 SG	172.57	130 N	129 CA	128 CG2	97.39
130 N	129 CA	61 NE2	81.36	130 N	129 CA	128 CG1	98.43
130 N	129 CA	131 N	29.69	130 N	129 CA	157 NH2	38.28
130 N	129 CA	156 N	115.10	130 N	129 CA	27 O	55.83

Fig. 11E

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 N	129 CA	61 ND1	100.25	130 N	129 CA	131 OG	57.41
130 N	129 CA	27 CD1	55.65	128 O	129 CA	301 OH2	80.40
128 O	129 CA	300 OH2	50.94	128 O	129 CA	128 CA	39.99
128 O	129 CA	130 CA	132.82	128 O	129 CA	128 CB	49.62
128 O	129 CA	130 C	145.78	128 O	129 CA	130 O	139.75
128 O	129 CA	128 N	26.80	128 O	129 CA	130 CB	117.84
128 O	129 CA	61 CE1	139.97	128 O	129 CA	152 SG	61.62
128 O	129 CA	128 CG2	40.41	128 O	129 CA	61 NE2	152.81
128 O	129 CA	128 CG1	60.51	128 O	129 CA	131 N	155.49
128 O	129 CA	157 NH2	111.44	128 O	129 CA	156 N	63.96
128 O	129 CA	27 O	70.79	128 O	129 CA	61 ND1	133.08
128 O	129 CA	131 OG	174.20	128 O	129 CA	27 CD1	81.81
301 OH2	129 CA	300 OH2	44.61	301 OH2	129 CA	128 CA	105.46
301 OH2	129 CA	130 CA	62.85	301 OH2	129 CA	128 CB	92.06
301 OH2	129 CA	130 C	67.04	301 OH2	129 CA	130 O	59.54
301 OH2	129 CA	128 N	101.56	301 OH2	129 CA	130 CB	50.15
301 OH2	129 CA	61 CE1	123.03	301 OH2	129 CA	152 SG	132.37
301 OH2	129 CA	128 CG2	78.34	301 OH2	129 CA	61 NE2	121.58
301 OH2	129 CA	128 CG1	101.18	301 OH2	129 CA	131 N	78.51
301 OH2	129 CA	157 NH2	32.72	301 OH2	129 CA	156 N	70.57
301 OH2	129 CA	27 O	21.79	301 OH2	129 CA	61 ND1	129.71
301 OH2	129 CA	131 OG	99.72	301 OH2	129 CA	27 CD1	65.65
300 OH2	129 CA	128 CA	90.09	300 OH2	129 CA	130 CA	106.66
300 OH2	129 CA	128 CB	92.04	300 OH2	129 CA	130 C	105.83
300 OH2	129 CA	130 O	93.27	300 OH2	129 CA	128 N	77.74
300 OH2	129 CA	130 CB	94.75	300 OH2	129 CA	61 CE1	120.91
300 OH2	129 CA	152 SG	87.94	300 OH2	129 CA	128 CG2	77.18
300 OH2	129 CA	61 NE2	132.46	300 OH2	129 CA	128 CG1	104.62
300 OH2	129 CA	131 N	117.07	300 OH2	129 CA	157 NH2	65.58

Fig. 11F

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
300 OH2	129 CA	156 N	32.29	300 OH2	129 CA	27 O	53.27
300 OH2	129 CA	61 ND1	121.41	300 OH2	129 CA	131 OG	125.51
300 OH2	129 CA	27 CD1	95.60	128 CA	129 CA	130 CA	121.64
128 CA	129 CA	128 CB	21.44	128 CA	129 CA	130 C	139.59
128 CA	129 CA	130 O	150.69	128 CA	129 CA	128 N	15.01
128 CA	129 CA	130 CB	113.43	128 CA	129 CA	61 CE1	131.37
128 CA	129 CA	152 SG	63.23	128 CA	129 CA	128 CG2	28.76
128 CA	129 CA	61 NE2	131.02	128 CA	129 CA	128 CG1	25.36
128 CA	129 CA	131 N	137.09	128 CA	129 CA	157 NH2	137.03
128 CA	129 CA	156 N	101.59	128 CA	129 CA	27 O	86.45
128 CA	129 CA	61 ND1	124.18	128 CA	129 CA	131 OG	144.28
128 CA	129 CA	27 CD1	65.91	130 CA	129 CA	128 CB	100.77
130 CA	129 CA	130 C	18.37	130 CA	129 CA	130 O	30.26
130 CA	129 CA	128 N	133.26	130 CA	129 CA	130 CB	15.25
130 CA	129 CA	61 CE1	86.73	130 CA	129 CA	152 SG	164.09
130 CA	129 CA	128 CG2	100.52	130 CA	129 CA	61 NE2	74.32
130 CA	129 CA	128 CG1	97.11	130 CA	129 CA	131 N	23.02
130 CA	129 CA	157 NH2	45.55	130 CA	129 CA	156 N	122.31
130 CA	129 CA	27 O	64.16	130 CA	129 CA	61 ND1	93.98
130 CA	129 CA	131 OG	51.03	130 CA	129 CA	27 CD1	57.24
128 CB	129 CA	130 C	119.05	128 CB	129 CA	130 O	129.25
128 CB	129 CA	128 N	33.01	128 CB	129 CA	130 CB	92.00
128 CB	129 CA	61 CE1	142.78	128 CB	129 CA	152 SG	84.64
128 CB	129 CA	128 CG2	15.54	128 CB	129 CA	61 NE2	135.21
128 CB	129 CA	128 CG1	12.58	128 CB	129 CA	131 N	118.84
128 CB	129 CA	157 NH2	119.85	128 CB	129 CA	156 N	113.35
128 CB	129 CA	27 O	70.86	128 CB	129 CA	61 ND1	137.61
128 CB	129 CA	131 OG	136.03	128 CB	129 CA	27 CD1	44.48
130 C	129 CA	130 O	15.09	130 C	129 CA	128 N	151.62

Fig. 11G

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 C	129 CA	130 CB	30.40	130 C	129 CA	61 CE1	71.14
130 C	129 CA	152 SG	151.30	130 C	129 CA	128 CG2	118.57
130 C	129 CA	61 NE2	60.78	130 C	129 CA	128 CG1	114.54
130 C	129 CA	131 N	11.59	130 C	129 CA	157 NH2	40.26
130 C	129 CA	156 N	111.69	130 C	129 CA	27 O	75.02
130 C	129 CA	61 ND1	78.83	130 C	129 CA	131 OG	36.51
130 C	129 CA	27 CD1	75.57	130 O	129 CA	128 N	157.77
130 O	129 CA	130 CB	37.27	130 O	129 CA	61 CE1	70.08
130 O	129 CA	152 SG	145.95	130 O	129 CA	128 CG2	124.77
130 O	129 CA	61 NE2	63.32	130 O	129 CA	128 CG1	127.20
130 O	129 CA	131 N	24.36	130 O	129 CA	157 NH2	28.62
130 O	129 CA	156 N	96.60	130 O	129 CA	27 O	72.57
130 O	129 CA	61 ND1	77.97	130 O	129 CA	131 OG	40.22
130 O	129 CA	27 CD1	84.78	128 N	129 CA	130 CB	122.37
128 N	129 CA	61 CE1	131.96	128 N	129 CA	152 SG	55.02
128 N	129 CA	128 CG2	33.67	128 N	129 CA	61 NE2	136.85
128 N	129 CA	128 CG1	39.79	128 N	129 CA	131 N	151.51
128 N	129 CA	157 NH2	134.26	128 N	129 CA	156 N	86.62
128 N	129 CA	27 O	85.93	128 N	129 CA	61 ND1	124.09
128 N	129 CA	131 OG	156.23	128 N	129 CA	27 CD1	76.06
130 CB	129 CA	61 CE1	101.15	130 CB	129 CA	152 SG	175.78
130 CB	129 CA	128 CG2	88.73	130 CB	129 CA	61 NE2	89.34
130 CB	129 CA	128 CG1	91.22	130 CB	129 CA	131 N	37.71
130 CB	129 CA	157 NH2	41.19	130 CB	129 CA	156 N	116.31
130 CB	129 CA	27 O	49.04	130 CB	129 CA	61 ND1	108.63
130 CB	129 CA	131 OG	65.67	130 CB	129 CA	27 CD1	47.53
61 CE1	129 CA	152 SG	80.17	61 CE1	129 CA	128 CG2	157.98
61 CE1	129 CA	61 NE2	15.28	61 CE1	129 CA	128 CG1	131.11
61 CE1	129 CA	131 N	63.71	61 CE1	129 CA	157 NH2	91.44

Fig. 11H

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CE1	129 CA	156 N	91.80	61 CE1	129 CA	27 O	141.74
61 CE1	129 CA	61 ND1	7.90	61 CE1	129 CA	131 OG	35.72
61 CE1	129 CA	27 CD1	135.69	152 SG	129 CA	128 CG2	88.69
152 SG	129 CA	61 NE2	91.25	152 SG	129 CA	128 CG1	84.94
152 SG	129 CA	131 N	142.89	152 SG	129 CA	157 NH2	143.00
152 SG	129 CA	156 N	67.51	152 SG	129 CA	27 O	131.52
152 SG	129 CA	61 ND1	72.53	152 SG	129 CA	131 OG	115.26
152 SG	129 CA	27 CD1	129.01	128 CG2	129 CA	61 NE2	150.34
128 CG2	129 CA	128 CG1	27.86	128 CG2	129 CA	131 N	121.91
128 CG2	129 CA	157 NH2	108.55	128 CG2	129 CA	156 N	101.46
128 CG2	129 CA	27 O	58.11	128 CG2	129 CA	61 ND1	151.95
128 CG2	129 CA	131 OG	145.36	128 CG2	129 CA	27 CD1	43.69
61 NE2	129 CA	128 CG1	122.66	61 NE2	129 CA	131 N	51.69
61 NE2	129 CA	157 NH2	88.87	61 NE2	129 CA	156 N	105.87
61 NE2	129 CA	27 O	135.44	61 NE2	129 CA	61 ND1	20.52
61 NE2	129 CA	131 OG	24.28	61 NE2	129 CA	27 CD1	120.42
128 CG1	129 CA	131 N	111.84	128 CG1	129 CA	157 NH2	125.19
128 CG1	129 CA	156 N	124.45	128 CG1	129 CA	27 O	79.45
128 CG1	129 CA	61 ND1	126.82	128 CG1	129 CA	131 OG	124.90
128 CG1	129 CA	27 CD1	44.91	131 N	129 CA	157 NH2	51.52
131 N	129 CA	156 N	119.25	131 N	129 CA	27 O	85.09
131 N	129 CA	61 ND1	71.01	131 N	129 CA	131 OG	28.03
131 N	129 CA	27 CD1	78.23	149 CA	129 CA	61 ND1	80.64
157 NH2	129 CA	156 N	76.91	157 NH2	129 CA	27 O	50.58
157 NH2	129 CA	61 ND1	98.77	157 NH2	129 CA	131 OG	67.78
157 NH2	129 CA	27 CD1	81.14	156 N	129 CA	27 O	84.43
156 N	129 CA	61 ND1	90.58	156 N	129 CA	131 OG	110.53
156 N	129 CA	27 CD1	127.86	27 O	129 CA	61 ND1	149.29
27 O	129 CA	131 OG	111.28	27 O	129 CA	27 CD1	46.17

Fig. 11I

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 ND1	129 CA	131 OG	42.99	61 ND1	129 CA	27 CD1	139.57
131 OG	129 CA	27 CD1	103.57	130 N	129 C	130 CA	31.03
130 N	129 C	130 C	44.35	130 N	129 C	128 C	114.04
130 N	129 C	130 O	42.82	130 N	129 C	130 CB	19.91
130 N	129 C	301 OH2	42.62	130 N	129 C	131 N	59.62
130 N	129 C	128 O	103.83	130 N	129 C	61 NE2	119.34
130 N	129 C	128 CA	117.36	130 N	129 C	148 O	81.79
130 N	129 C	61 CE1	123.79	130 N	129 C	300 OH2	77.83
130 N	129 C	128 CB	102.79	130 N	129 C	131 OG	90.42
130 N	129 C	130 CG	27.54	130 N	129 C	131 CA	64.03
130 N	129 C	157 NH2	28.97	130 N	129 C	130 CD1	42.98
130 N	129 C	27 CD1	63.27	130 N	129 C	148 C	89.12
130 N	129 C	128 CG1	107.50	130 N	129 C	128 CG2	91.90
130 N	129 C	131 CB	79.27	130 N	129 C	61 CD2	123.37
130 N	129 C	128 N	115.99	130 N	129 C	61 ND1	129.60
130 N	129 C	27 O	39.51	130 CA	129 C	130 C	26.56
130 CA	129 C	128 C	137.39	130 CA	129 C	130 O	39.60
130 CA	129 C	130 CB	17.13	130 CA	129 C	301 OH2	73.65
130 CA	129 C	131 N	34.38	130 CA	129 C	128 O	132.43
130 CA	129 C	61 NE2	99.29	130 CA	129 C	128 CA	133.32
130 CA	129 C	148 O	50.83	130 CA	129 C	61 CE1	110.86
130 CA	129 C	300 OH2	108.66	130 CA	129 C	128 CB	114.56
130 CA	129 C	131 OG	69.13	130 CA	129 C	130 CG	7.26
130 CA	129 C	131 CA	42.82	130 CA	129 C	157 NH2	49.39
130 CA	129 C	130 CD1	17.50	130 CA	129 C	27 CD1	66.85
130 CA	129 C	148 C	58.69	130 CA	129 C	128 CG1	111.76
130 CA	129 C	128 CG2	108.48	130 CA	129 C	131 CB	56.14
130 CA	129 C	61 CD2	100.32	130 CA	129 C	128 N	136.88
130 CA	129 C	61 ND1	115.62	130 CA	129 C	27 O	66.79

Fig. 11J

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 C	129 C	128 C	158.17	130 C	129 C	130 O	18.93
130 C	129 C	130 CB	41.05	130 C	129 C	301 OH2	81.01
130 C	129 C	131 N	17.29	130 C	129 C	128 O	144.59
130 C	129 C	61 NE2	76.44	130 C	129 C	128 CA	159.47
130 C	129 C	148 O	52.05	130 C	129 C	61 CE1	85.54
130 C	129 C	300 OH2	109.33	130 C	129 C	128 CB	141.05
130 C	129 C	131 OG	46.45	130 C	129 C	130 CG	33.42
130 C	129 C	131 CA	19.68	130 C	129 C	157 NH2	44.37
130 C	129 C	130 CD1	40.52	130 C	129 C	27 CD1	93.41
130 C	129 C	148 C	62.15	130 C	129 C	128 CG1	137.68
130 C	129 C	128 CG2	133.67	130 C	129 C	131 CB	34.92
130 C	129 C	61 CD2	79.40	130 C	129 C	128 N	160.30
130 C	129 C	61 ND1	90.76	130 C	129 C	27 O	83.83
128 C	129 C	130 O	145.98	128 C	129 C	130 CB	120.61
128 C	129 C	301 OH2	77.98	128 C	129 C	131 N	171.40
128 C	129 C	128 O	17.11	128 C	129 C	61 NE2	123.21
128 C	129 C	128 CA	14.44	128 C	129 C	148 O	140.12
128 C	129 C	61 CE1	111.33	128 C	129 C	300 OH2	54.23
128 C	129 C	128 CB	29.26	128 C	129 C	131 OG	153.47
128 C	129 C	130 CG	130.17	128 C	129 C	131 CA	175.37
128 C	129 C	157 NH2	116.37	128 C	129 C	130 CD1	130.04
128 C	129 C	27 CD1	74.34	128 C	129 C	148 C	130.33
128 C	129 C	128 CG1	39.65	128 C	129 C	128 CG2	30.19
128 C	129 C	131 CB	166.26	128 C	129 C	61 CD2	121.36
128 C	129 C	128 N	5.25	128 C	129 C	61 ND1	106.87
128 C	129 C	27 O	74.53	130 O	129 C	130 CB	48.72
130 O	129 C	301 OH2	69.31	130 O	129 C	131 N	33.52
130 O	129 C	128 O	129.39	130 O	129 C	61 NE2	77.19
130 O	129 C	128 CA	156.66	130 O	129 C	148 O	70.22

Fig. 11K

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 O	129 C	61 CE1	81.26	130 O	129 C	300 OH2	92.47
130 O	129 C	128 CB	145.53	130 O	129 C	131 OG	50.94
130 O	129 C	130 CG	44.80	130 O	129 C	131 CA	29.88
130 O	129 C	157 NH2	30.07	130 O	129 C	130 CD1	56.26
130 O	129 C	27 CD1	102.76	130 O	129 C	148 C	80.40
130 O	129 C	128 CG1	149.06	130 O	129 C	128 CG2	133.87
130 O	129 C	131 CB	43.34	130 O	129 C	61 CD2	82.31
130 O	129 C	128 N	150.53	130 O	129 C	61 ND1	87.02
130 O	129 C	27 O	78.84	130 CB	129 C	301 OH2	60.34
130 CB	129 C	131 N	51.35	130 CB	129 C	128 O	115.50
130 CB	129 C	61 NE2	116.18	130 CB	129 C	128 CA	118.42
130 CB	129 C	148 O	64.37	130 CB	129 C	61 CE1	126.60
130 CB	129 C	300 OH2	95.98	130 CB	129 C	128 CB	100.46
130 CB	129 C	131 OG	85.88	130 CB	129 C	130 CG	10.52
130 CB	129 C	131 CA	59.14	130 CB	129 C	157 NH2	46.52
130 CB	129 C	130 CD1	23.55	130 CB	129 C	27 CD1	54.17
130 CB	129 C	148 C	70.54	130 CB	129 C	128 CG1	100.49
130 CB	129 C	128 CG2	92.71	130 CB	129 C	131 CB	73.05
130 CB	129 C	61 CD2	117.44	130 CB	129 C	128 N	120.63
130 CB	129 C	61 ND1	131.74	130 CB	129 C	27 O	50.20
301 OH2	129 C	131 N	98.20	301 OH2	129 C	128 O	63.83
301 OH2	129 C	61 NE2	134.42	301 OH2	129 C	128 CA	87.40
301 OH2	129 C	148 O	124.32	301 OH2	129 C	61 CE1	124.57
301 OH2	129 C	300 OH2	35.64	301 OH2	129 C	128 CB	82.32
301 OH2	129 C	131 OG	118.78	301 OH2	129 C	130 CG	69.67
301 OH2	129 C	131 CA	98.52	301 OH2	129 C	157 NH2	39.32
301 OH2	129 C	130 CD1	83.74	301 OH2	129 C	27 CD1	71.31
301 OH2	129 C	148 C	130.85	301 OH2	129 C	128 CG1	94.19
301 OH2	129 C	128 CG2	69.24	301 OH2	129 C	131 CB	112.65

Fig. 11L

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
301 OH2	129 C	61 CD2	142.03	301 OH2	129 C	128 N	81.78
301 OH2	129 C	61 ND1	128.19	301 OH2	129 C	27 O	23.32
131 N	129 C	128 O	161.88	131 N	129 C	61 NE2	64.91
131 N	129 C	128 CA	160.40	131 N	129 C	148 O	37.05
131 N	129 C	61 CE1	77.21	131 N	129 C	300 OH2	125.87
131 N	129 C	128 CB	143.16	131 N	129 C	131 OG	34.84
131 N	129 C	130 CG	41.55	131 N	129 C	131 CA	10.79
131 N	129 C	157 NH2	61.43	131 N	129 C	130 CD1	41.43
131 N	129 C	27 CD1	97.18	131 N	129 C	148 C	47.21
131 N	129 C	128 CG1	134.19	131 N	129 C	128 CG2	141.24
131 N	129 C	131 CB	21.78	131 N	129 C	61 CD2	66.25
131 N	129 C	128 N	168.62	131 N	129 C	61 ND1	81.58
131 N	129 C	27 O	98.87	128 O	129 C	61 NE2	125.36
128 O	129 C	128 CA	31.18	128 O	129 C	148 O	156.02
128 O	129 C	61 CE1	110.32	128 O	129 C	300 OH2	37.16
128 O	129 C	128 CB	41.91	128 O	129 C	131 OG	151.33
128 O	129 C	130 CG	125.98	128 O	129 C	131 CA	158.30
128 O	129 C	157 NH2	100.59	128 O	129 C	130 CD1	131.96
128 O	129 C	27 CD1	79.76	128 O	129 C	148 C	146.82
128 O	129 C	128 CG1	54.37	128 O	129 C	128 CG2	37.30
128 O	129 C	131 CB	162.05	128 O	129 C	61 CD2	126.20
128 O	129 C	128 N	22.28	128 O	129 C	61 ND1	107.23
128 O	129 C	27 O	65.71	61 NE2	129 C	128 CA	123.13
61 NE2	129 C	148 O	67.59	61 NE2	129 C	61 CE1	16.57
61 NE2	129 C	300 OH2	120.67	61 NE2	129 C	128 CB	137.09
61 NE2	129 C	131 OG	30.33	61 NE2	129 C	130 CG	106.45
61 NE2	129 C	131 CA	57.28	61 NE2	129 C	157 NH2	101.97
61 NE2	129 C	130 CD1	102.68	61 NE2	129 C	27 CD1	148.17
61 NE2	129 C	148 C	69.34	61 NE2	129 C	128 CG1	128.64

Fig. 11M

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 NE2	129 C	128 CG2	148.74	61 NE2	129 C	131 CB	43.15
61 NE2	129 C	61 CD2	7.65	61 NE2	129 C	128 N	122.88
61 NE2	129 C	61 ND1	18.29	61 NE2	129 C	27 O	154.32
128 CA	129 C	148 O	125.68	128 CA	129 C	61 CE1	114.97
128 CA	129 C	300 OH2	67.87	128 CA	129 C	128 CB	18.95
128 CA	129 C	131 OG	151.80	128 CA	129 C	130 CG	126.26
128 CA	129 C	131 CA	170.11	128 CA	129 C	157 NH2	126.71
128 CA	129 C	130 CD1	121.61	128 CA	129 C	27 CD1	66.72
128 CA	129 C	148 C	115.92	128 CA	129 C	128 CG1	26.22
128 CA	129 C	128 CG2	26.02	128 CA	129 C	131 CB	159.86
128 CA	129 C	61 CD2	119.20	128 CA	129 C	128 N	9.24
128 CA	129 C	61 ND1	109.69	128 CA	129 C	27 O	78.95
148 O	129 C	61 CE1	84.13	148 O	129 C	300 OH2	159.40
148 O	129 C	128 CB	114.25	148 O	129 C	131 OG	49.48
148 O	129 C	130 CG	54.69	148 O	129 C	131 CA	44.46
148 O	129 C	157 NH2	95.27	148 O	129 C	130 CD1	41.74
148 O	129 C	27 CD1	82.28	148 O	129 C	148 C	10.19
148 O	129 C	128 CG1	101.66	148 O	129 C	128 CG2	120.43
148 O	129 C	131 CB	41.34	148 O	129 C	61 CD2	63.68
148 O	129 C	128 N	134.90	148 O	129 C	61 ND1	85.33
148 O	129 C	27 O	112.25	61 CE1	129 C	300 OH2	104.76
61 CE1	129 C	128 CB	132.38	61 CE1	129 C	131 OG	42.66
61 CE1	129 C	130 CG	118.11	61 CE1	129 C	131 CA	68.06
61 CE1	129 C	157 NH2	100.17	61 CE1	129 C	130 CD1	117.31
61 CE1	129 C	27 CD1	163.49	61 CE1	129 C	148 C	85.80
61 CE1	129 C	128 CG1	128.63	61 CE1	129 C	128 CG2	140.60
61 CE1	129 C	131 CB	55.79	61 CE1	129 C	61 CD2	21.94
61 CE1	129 C	128 N	112.26	61 CE1	129 C	61 ND1	5.81
61 CE1	129 C	27 O	147.66	300 OH2	129 C	128 CB	73.67

Fig. 11N

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
300 OH2	129 C	131 OG	127.21	300 OH2	129 C	130 CG	105.20
300 OH2	129 C	131 CA	121.23	300 OH2	129 C	157 NH2	65.15
300 OH2	129 C	130 CD1	119.30	300 OH2	129 C	27 CD1	91.15
300 OH2	129 C	148 C	166.33	300 OH2	129 C	128 CG1	87.40
300 OH2	129 C	128 CG2	63.67	300 OH2	129 C	131 CB	129.90
300 OH2	129 C	61 CD2	126.69	300 OH2	129 C	128 N	59.32
300 OH2	129 C	61 ND1	105.42	300 OH2	129 C	27 O	51.39
128 CB	129 C	131 OG	157.80	128 CB	129 C	130 CG	107.63
128 CB	129 C	131 CA	153.95	128 CB	129 C	157 NH2	119.83
128 CB	129 C	130 CD1	102.79	128 CB	129 C	27 CD1	47.80
128 CB	129 C	148 C	105.81	128 CB	129 C	128 CG1	13.78
128 CB	129 C	128 CG2	13.10	128 CB	129 C	131 CB	155.44
128 CB	129 C	61 CD2	131.38	128 CB	129 C	128 N	25.47
128 CB	129 C	61 ND1	126.78	128 CB	129 C	27 O	67.78
131 OG	129 C	130 CG	76.34	131 OG	129 C	131 CA	27.01
131 OG	129 C	157 NH2	79.91	131 OG	129 C	130 CD1	74.80
131 OG	129 C	27 CD1	128.86	131 OG	129 C	148 C	56.01
131 OG	129 C	128 CG1	144.27	131 OG	129 C	128 CG2	169.11
131 OG	129 C	131 CB	13.16	131 OG	129 C	61 CD2	33.00
131 OG	129 C	128 N	153.12	131 OG	129 C	61 ND1	46.79
131 OG	129 C	27 O	129.24	130 CG	129 C	131 CA	50.07
130 CG	129 C	157 NH2	49.98	130 CG	129 C	130 CD1	16.17
130 CG	129 C	27 CD1	60.07	130 CG	129 C	148 C	61.60
130 CG	129 C	128 CG1	105.57	130 CG	129 C	128 CG2	101.25
130 CG	129 C	131 CB	63.33	130 CG	129 C	61 CD2	107.24
130 CG	129 C	128 N	129.62	130 CG	129 C	61 ND1	122.87
130 CG	129 C	27 O	60.70	131 CA	129 C	157 NH2	59.75
131 CA	129 C	130 CD1	51.84	131 CA	129 C	27 CD1	107.57
131 CA	129 C	148 C	54.29	131 CA	129 C	128 CG1	144.43

Fig. 110

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
131 CA	129 C	128 CG2	151.13	131 CA	129 C	131 CB	15.28
131 CA	129 C	61 CD2	59.81	131 CA	129 C	128 N	179.34
131 CA	129 C	61 ND1	72.82	131 CA	129 C	27 O	103.46
157 NH2	129 C	130 CD1	65.98	157 NH2	129 C	27 CD1	90.38
157 NH2	129 C	148 C	104.90	157 NH2	129 C	128 CG1	129.35
157 NH2	129 C	128 CG2	106.87	157 NH2	129 C	131 CB	73.38
157 NH2	129 C	61 CD2	108.47	157 NH2	129 C	128 N	120.62
157 NH2	129 C	61 ND1	105.75	157 NH2	129 C	27 O	52.43
130 CD1	129 C	27 CD1	55.76	130 CD1	129 C	148 C	47.11
130 CD1	129 C	128 CG1	97.25	130 CD1	129 C	128 CG2	99.87
130 CD1	129 C	131 CB	61.81	130 CD1	129 C	61 CD2	101.36
130 CD1	129 C	128 N	127.67	130 CD1	129 C	61 ND1	120.76
130 CD1	129 C	27 O	70.80	27 CD1	129 C	148 C	79.20
27 CD1	129 C	128 CG1	46.34	27 CD1	129 C	128 CG2	44.27
27 CD1	129 C	131 CB	116.63	27 CD1	129 C	61 CD2	141.87
27 CD1	129 C	128 N	71.96	27 CD1	129 C	61 ND1	160.49
27 CD1	129 C	27 O	47.99	148 C	129 C	128 CG1	92.74
148 C	129 C	128 CG2	113.38	148 C	129 C	131 CB	49.63
148 C	129 C	61 CD2	64.24	148 C	129 C	128 N	125.09
148 C	129 C	61 ND1	85.97	148 C	129 C	27 O	115.37
128 CG1	129 C	128 CG2	25.68	128 CG1	129 C	131 CB	142.19
128 CG1	129 C	61 CD2	121.89	128 CG1	129 C	128 N	34.92
128 CG1	129 C	61 ND1	122.82	128 CG1	129 C	27 O	77.02
128 CG2	129 C	131 CB	160.37	128 CG2	129 C	61 CD2	143.80
128 CG2	129 C	128 N	28.50	128 CG2	129 C	61 ND1	135.54
128 CG2	129 C	27 O	55.23	131 CB	129 C	61 CD2	44.92
131 CB	129 C	128 N	164.64	131 CB	129 C	61 ND1	59.93
131 CB	129 C	27 O	118.74	61 CD2	129 C	128 N	120.26
61 CD2	129 C	61 ND1	21.79	61 CD2	129 C	27 O	160.83

Fig. 11P

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 N	129 C	61 ND1	107.46	128 N	129 C	27 O	76.58
61 ND1	129 C	27 O	151.51	130 N	129 O	130 CA	31.92
130 N	129 O	130 C	46.12	130 N	129 O	131 N	66.02
130 N	129 O	61 NE2	118.69	130 N	129 O	148 O	96.55
130 N	129 O	130 O	41.64	130 N	129 O	128 C	76.90
130 N	129 O	130 CB	29.28	130 N	129 O	61 CE1	112.75
130 N	129 O	131 OG	95.89	130 N	129 O	148 C	107.17
130 N	129 O	61 CD2	129.64	130 N	129 O	128 O	67.81
130 N	129 O	301 OH2	19.06	130 N	129 O	131 CA	72.00
130 N	129 O	128 CA	86.79	130 N	129 O	128 CB	79.07
130 N	129 O	131 CB	88.76	130 N	129 O	130 CG	41.07
130 N	129 O	61 ND1	120.73	130 N	129 O	130 CD1	56.16
130 N	129 O	148 ND1	132.58	130 N	129 O	128 CG1	90.05
130 N	129 O	61 CG	130.10	130 N	129 O	148 CE1	130.24
130 N	129 O	300 OH2	46.46	130 N	129 O	27 CD1	58.05
130 CA	129 O	130 C	25.78	130 CA	129 O	131 N	39.77
130 CA	129 O	61 NE2	110.68	130 CA	129 O	148 O	64.67
130 CA	129 O	130 O	33.92	130 CA	129 O	128 C	105.56
130 CA	129 O	130 CB	10.28	130 CA	129 O	61 CE1	115.51
130 CA	129 O	131 OG	77.83	130 CA	129 O	148 C	75.92
130 CA	129 O	61 CD2	116.75	130 CA	129 O	128 O	98.44
130 CA	129 O	301 OH2	50.97	130 CA	129 O	131 CA	49.39
130 CA	129 O	128 CA	111.40	130 CA	129 O	128 CB	98.09
130 CA	129 O	131 CB	66.13	130 CA	129 O	130 CG	10.68
130 CA	129 O	61 ND1	123.22	130 CA	129 O	130 CD1	27.04
130 CA	129 O	148 ND1	102.02	130 CA	129 O	128 CG1	103.22
130 CA	129 O	61 CG	124.02	130 CA	129 O	148 CE1	103.04
130 CA	129 O	300 OH2	78.25	130 CA	129 O	27 CD1	59.76
130 C	129 O	131 N	20.56	130 C	129 O	61 NE2	84.94

Fig. 11Q

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 C	129 O	148 O	61.06	130 C	129 O	130 O	15.29
130 C	129 O	128 C	122.50	130 C	129 O	130 CB	36.03
130 C	129 O	61 CE1	90.54	130 C	129 O	131 OG	53.09
130 C	129 O	148 C	74.74	130 C	129 O	61 CD2	91.71
130 C	129 O	128 O	111.97	130 C	129 O	301 OH2	62.80
130 C	129 O	131 CA	26.14	130 C	129 O	128 CA	132.80
130 C	129 O	128 CB	122.40	130 C	129 O	131 CB	43.24
130 C	129 O	130 CG	30.55	130 C	129 O	61 ND1	97.90
130 C	129 O	130 CD1	41.63	130 C	129 O	148 ND1	87.51
130 C	129 O	128 CG1	128.93	130 C	129 O	61 CG	98.30
130 C	129 O	148 CE1	84.14	130 C	129 O	300 OH2	85.09
130 C	129 O	27 CD1	85.46	131 N	129 O	61 NE2	74.34
131 N	129 O	148 O	43.59	131 N	129 O	130 O	32.60
131 N	129 O	128 C	142.86	131 N	129 O	130 CB	49.34
131 N	129 O	61 CE1	85.19	131 N	129 O	131 OG	39.67
131 N	129 O	148 C	57.34	131 N	129 O	61 CD2	77.95
131 N	129 O	128 O	132.52	131 N	129 O	301 OH2	83.28
131 N	129 O	131 CA	11.61	131 N	129 O	128 CA	151.15
131 N	129 O	128 CB	136.98	131 N	129 O	131 CB	26.64
131 N	129 O	130 CG	38.83	131 N	129 O	61 ND1	90.86
131 N	129 O	130 CD1	41.59	131 N	129 O	148 ND1	67.05
131 N	129 O	128 CG1	137.92	131 N	129 O	61 CG	86.86
131 N	129 O	148 CE1	64.68	131 N	129 O	300 OH2	105.17
131 N	129 O	27 CD1	94.15	61 NE2	129 O	148 O	83.76
61 NE2	129 O	130 O	80.78	61 NE2	129 O	128 C	125.31
61 NE2	129 O	130 CB	120.95	61 NE2	129 O	61 CE1	17.95
61 NE2	129 O	131 OG	34.77	61 NE2	129 O	148 C	86.45
61 NE2	129 O	61 CD2	12.11	61 NE2	129 O	128 O	120.84
61 NE2	129 O	301 OH2	119.92	61 NE2	129 O	131 CA	63.06

Fig. 11R

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 NE2	129 O	128 CA	130.56	61 NE2	129 O	128 CB	147.76
61 NE2	129 O	131 CB	48.75	61 NE2	129 O	130 CG	112.83
61 NE2	129 O	61 ND1	18.56	61 NE2	129 O	130 CD1	114.07
61 NE2	129 O	148 ND1	52.08	61 NE2	129 O	128 CG1	146.09
61 NE2	129 O	61 CG	13.39	61 NE2	129 O	148 CE1	39.43
61 NE2	129 O	300 OH2	109.53	61 NE2	129 O	27 CD1	167.74
148 O	129 O	130 O	75.45	148 O	129 O	128 C	149.99
148 O	129 O	130 CB	68.50	148 O	129 O	61 CE1	101.39
148 O	129 O	131 OG	58.31	148 O	129 O	148 C	13.80
148 O	129 O	61 CD2	78.29	148 O	129 O	128 O	154.77
148 O	129 O	301 OH2	115.51	148 O	129 O	131 CA	48.65
148 O	129 O	128 CA	138.21	148 O	129 O	128 CB	122.94
148 O	129 O	131 CB	46.79	148 O	129 O	130 CG	55.74
148 O	129 O	61 ND1	101.63	148 O	129 O	130 CD1	42.71
148 O	129 O	148 ND1	41.41	148 O	129 O	128 CG1	112.21
148 O	129 O	61 CG	89.57	148 O	129 O	148 CE1	49.18
148 O	129 O	300 OH2	142.90	148 O	129 O	27 CD1	84.94
130 O	129 O	128 C	113.15	130 O	129 O	130 CB	42.97
130 O	129 O	61 CE1	82.12	130 O	129 O	131 OG	54.25
130 O	129 O	148 C	89.24	130 O	129 O	61 CD2	89.93
130 O	129 O	128 O	101.36	130 O	129 O	301 OH2	54.65
130 O	129 O	131 CA	33.29	130 O	129 O	128 CA	126.21
130 O	129 O	128 CB	120.68	130 O	129 O	131 CB	48.47
130 O	129 O	130 CG	41.90	130 O	129 O	61 ND1	90.14
130 O	129 O	130 CD1	55.39	130 O	129 O	148 ND1	96.39
130 O	129 O	128 CG1	131.16	130 O	129 O	61 CG	93.91
130 O	129 O	148 CE1	90.23	130 O	129 O	300 OH2	72.96
130 O	129 O	27 CD1	91.80	128 C	129 O	130 CB	97.59
128 C	129 O	61 CE1	108.18	128 C	129 O	131 OG	150.60

Fig. 11S

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 C	129 O	148 C	142.41	128 C	129 O	61 CD2	128.48
128 C	129 O	128 O	12.64	128 C	129 O	301 OH2	59.72
128 C	129 O	131 CA	146.43	128 C	129 O	128 CA	15.50
128 C	129 O	128 CB	27.35	128 C	129 O	131 CB	158.26
128 C	129 O	130 CG	110.33	128 C	129 O	61 ND1	106.89
128 C	129 O	130 CD1	116.84	128 C	129 O	148 ND1	149.96
128 C	129 O	128 CG1	39.77	128 C	129 O	61 CG	117.27
128 C	129 O	148 CE1	151.38	128 C	129 O	300 OH2	41.54
128 C	129 O	27 CD1	66.59	130 CB	129 O	61 CE1	125.06
130 CB	129 O	131 OG	87.97	130 CB	129 O	148 C	78.13
130 CB	129 O	61 CD2	126.87	130 CB	129 O	128 O	91.86
130 CB	129 O	301 OH2	47.44	130 CB	129 O	131 CA	59.40
130 CB	129 O	128 CA	102.01	130 CB	129 O	128 CB	88.07
130 CB	129 O	131 CB	75.91	130 CB	129 O	130 CG	13.16
130 CB	129 O	61 ND1	132.97	130 CB	129 O	130 CD1	26.91
130 CB	129 O	148 ND1	108.21	130 CB	129 O	128 CG1	92.95
130 CB	129 O	61 CG	134.30	130 CB	129 O	148 CE1	110.96
130 CB	129 O	300 OH2	75.18	130 CB	129 O	27 CD1	49.67
61 CE1	129 O	131 OG	47.94	61 CE1	129 O	148 C	104.39
61 CE1	129 O	61 CD2	27.14	61 CE1	129 O	128 O	102.94
61 CE1	129 O	301 OH2	108.32	61 CE1	129 O	131 CA	73.59
61 CE1	129 O	128 CA	115.65	61 CE1	129 O	128 CB	133.11
61 CE1	129 O	131 CB	62.25	61 CE1	129 O	130 CG	120.87
61 CE1	129 O	61 ND1	8.26	61 CE1	129 O	130 CD1	126.72
61 CE1	129 O	148 ND1	69.27	61 CE1	129 O	128 CG1	136.86
61 CE1	129 O	61 CG	19.41	61 CE1	129 O	148 CE1	56.95
61 CE1	129 O	300 OH2	93.11	61 CE1	129 O	27 CD1	169.74
131 OG	129 O	148 C	66.99	131 OG	129 O	61 CD2	38.92
131 OG	129 O	128 O	139.72	131 OG	129 O	301 OH2	106.95

Fig. 11T

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
131 OG	129 O	131 CA	28.69	131 OG	129 O	128 CA	162.98
131 OG	129 O	128 CB	174.85	131 OG	129 O	131 CB	14.34
131 OG	129 O	130 CG	78.43	131 OG	129 O	61 ND1	52.19
131 OG	129 O	130 CD1	79.66	131 OG	129 O	148 ND1	48.31
131 OG	129 O	128 CG1	169.27	131 OG	129 O	61 CG	47.21
131 OG	129 O	148 CE1	38.19	131 OG	129 O	300 OH2	114.22
131 OG	129 O	27 CD1	133.38	148 C	129 O	61 CD2	78.56
148 C	129 O	128 O	151.78	148 C	129 O	301 OH2	125.52
148 C	129 O	131 CA	61.75	148 C	129 O	128 CA	128.24
148 C	129 O	128 CB	115.32	148 C	129 O	131 CB	57.44
148 C	129 O	130 CG	66.15	148 C	129 O	61 ND1	102.62
148 C	129 O	130 CD1	51.29	148 C	129 O	148 ND1	37.29
148 C	129 O	128 CG1	102.73	148 C	129 O	61 CG	89.23
148 C	129 O	148 CE1	48.09	148 C	129 O	300 OH2	153.18
148 C	129 O	27 CD1	83.69	61 CD2	129 O	128 O	126.93
61 CD2	129 O	301 OH2	132.02	61 CD2	129 O	131 CA	67.49
61 CD2	129 O	128 CA	129.67	61 CD2	129 O	128 CB	145.00
61 CD2	129 O	131 CB	51.35	61 CD2	129 O	130 CG	116.67
61 CD2	129 O	61 ND1	24.07	61 CD2	129 O	130 CD1	114.18
61 CD2	129 O	148 ND1	42.30	61 CD2	129 O	128 CG1	138.67
61 CD2	129 O	61 CG	11.34	61 CD2	129 O	148 CE1	30.48
61 CD2	129 O	300 OH2	120.22	61 CD2	129 O	27 CD1	162.14
128 O	129 O	301 OH2	49.54	128 O	129 O	131 CA	134.39
128 O	129 O	128 CA	28.06	128 O	129 O	128 CB	37.20
128 O	129 O	131 CB	145.69	128 O	129 O	130 CG	105.01
128 O	129 O	61 ND1	103.41	128 O	129 O	130 CD1	114.72
128 O	129 O	148 ND1	159.49	128 O	129 O	128 CG1	50.96
128 O	129 O	61 CG	115.66	128 O	129 O	148 CE1	155.49
128 O	129 O	300 OH2	29.01	128 O	129 O	27 CD1	70.04

Fig. 11U

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
301 OH2	129 O	131 CA	87.46	301 OH2	129 O	128 CA	71.61
301 OH2	129 O	128 CB	67.92	301 OH2	129 O	131 CB	103.12
301 OH2	129 O	130 CG	59.84	301 OH2	129 O	61 ND1	115.06
301 OH2	129 O	130 CD1	74.23	301 OH2	129 O	148 ND1	150.31
301 OH2	129 O	128 CG1	81.28	301 OH2	129 O	61 CG	127.66
301 OH2	129 O	148 CE1	144.66	301 OH2	129 O	300 OH2	27.74
301 OH2	129 O	27 CD1	61.47	131 CA	129 O	128 CA	158.78
131 CA	129 O	128 CB	147.47	131 CA	129 O	131 CB	17.14
131 CA	129 O	130 CG	49.83	131 CA	129 O	61 ND1	79.29
131 CA	129 O	130 CD1	53.17	131 CA	129 O	148 ND1	63.18
131 CA	129 O	128 CG1	149.52	131 CA	129 O	61 CG	75.83
131 CA	129 O	148 CE1	58.29	131 CA	129 O	300 OH2	105.54
131 CA	129 O	27 CD1	105.62	128 CA	129 O	128 CB	17.49
128 CA	129 O	131 CB	173.75	128 CA	129 O	130 CG	113.39
128 CA	129 O	61 ND1	112.28	128 CA	129 O	130 CD1	115.26
128 CA	129 O	148 ND1	137.23	128 CA	129 O	128 CG1	26.00
128 CA	129 O	61 CG	119.60	128 CA	129 O	148 CE1	142.93
128 CA	129 O	300 OH2	56.64	128 CA	129 O	27 CD1	61.68
128 CB	129 O	131 CB	163.36	128 CB	129 O	130 CG	98.16
128 CB	129 O	61 ND1	129.69	128 CB	129 O	130 CD1	98.17
128 CB	129 O	148 ND1	136.37	128 CB	129 O	128 CG1	14.81
128 CB	129 O	61 CG	136.00	128 CB	129 O	148 CE1	146.84
128 CB	129 O	300 OH2	61.50	128 CB	129 O	27 CD1	44.39
131 CB	129 O	130 CG	65.34	131 CB	129 O	61 ND1	66.47
131 CB	129 O	130 CD1	65.43	131 CB	129 O	148 ND1	48.52
131 CB	129 O	128 CG1	158.56	131 CB	129 O	61 CG	60.64
131 CB	129 O	148 CE1	41.85	131 CB	129 O	300 OH2	117.15
131 CB	129 O	27 CD1	119.22	130 CG	129 O	61 ND1	127.86
130 CG	129 O	130 CD1	16.36	130 CG	129 O	148 ND1	95.05

Fig. 11V

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 CG	129 O	128 CG1	100.61	130 CG	129 O	61 CG	125.63
130 CG	129 O	148 CE1	98.07	130 CG	129 O	300 OH2	87.50
130 CG	129 O	27 CD1	56.26	61 ND1	129 O	130 CD1	131.84
61 ND1	129 O	148 ND1	66.10	61 ND1	129 O	128 CG1	131.09
61 ND1	129 O	61 CG	13.95	61 ND1	129 O	148 CE1	54.54
61 ND1	129 O	300 OH2	97.43	61 ND1	129 O	27 CD1	173.42
130 CD1	129 O	148 ND1	83.88	130 CD1	129 O	128 CG1	96.41
130 CD1	129 O	61 CG	124.92	130 CD1	129 O	148 CE1	89.66
130 CD1	129 O	300 OH2	101.92	130 CD1	129 O	27 CD1	53.81
148 ND1	129 O	128 CG1	121.62	148 ND1	129 O	61 CG	52.34
148 ND1	129 O	148 CE1	12.95	148 ND1	129 O	300 OH2	160.82
148 ND1	129 O	27 CD1	119.87	128 CG1	129 O	61 CG	132.75
128 CG1	129 O	148 CE1	132.56	128 CG1	129 O	300 OH2	76.28
128 CG1	129 O	27 CD1	44.35	61 CG	129 O	148 CE1	41.23
61 CG	129 O	300 OH2	111.38	61 CG	129 O	27 CD1	170.85
148 CE1	129 O	300 OH2	147.94	148 CE1	129 O	27 CD1	131.71
300 OH2	129 O	27 CD1	77.16	128 C	129 CB	128 O	21.26
128 C	129 CB	130 N	78.75	128 C	129 CB	61 CE1	158.28
128 C	129 CB	152 SG	72.13	128 C	129 CB	300 OH2	62.18
128 C	129 CB	61 NE2	143.34	128 C	129 CB	128 CA	12.60
128 C	129 CB	61 ND1	154.13	128 C	129 CB	301 OH2	67.63
128 C	129 CB	130 CA	86.83	128 C	129 CB	130 C	103.49
128 C	129 CB	130 O	108.89	128 C	129 CB	152 CB	83.75
128 C	129 CB	128 N	16.24	128 C	129 CB	128 CB	15.97
128 C	129 CB	61 CD2	140.03	128 C	129 CB	156 N	89.39
128 C	129 CB	61 CG	145.70	128 C	129 CB	131 OG	134.35
128 C	129 CB	131 N	109.25	128 C	129 CB	152 N	65.83
128 C	129 CB	130 CB	79.86	128 O	129 CB	130 N	81.98
128 O	129 CB	61 CE1	179.39	128 O	129 CB	152 SG	71.44

Fig. 11W

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 O	129 CB	300 OH2	42.67	128 O	129 CB	61 NE2	162.18
128 O	129 CB	128 CA	32.55	128 O	129 CB	61 ND1	167.04
128 O	129 CB	301 OH2	58.17	128 O	129 CB	130 CA	92.11
128 O	129 CB	130 C	106.53	128 O	129 CB	130 O	106.85
128 O	129 CB	152 CB	86.64	128 O	129 CB	128 N	25.60
128 O	129 CB	128 CB	35.75	128 O	129 CB	61 CD2	161.09
128 O	129 CB	156 N	68.34	128 O	129 CB	61 CG	165.19
128 O	129 CB	131 OG	143.85	128 O	129 CB	131 N	115.69
128 O	129 CB	152 N	75.48	128 O	129 CB	130 CB	83.10
130 N	129 CB	61 CE1	98.32	130 N	129 CB	152 SG	150.85
130 N	129 CB	300 OH2	72.80	130 N	129 CB	61 NE2	84.22
130 N	129 CB	128 CA	84.43	130 N	129 CB	61 ND1	110.43
130 N	129 CB	301 OH2	37.74	130 N	129 CB	130 CA	10.85
130 N	129 CB	130 C	25.08	130 N	129 CB	130 O	31.37
130 N	129 CB	152 CB	157.85	130 N	129 CB	128 N	94.97
130 N	129 CB	128 CB	69.07	130 N	129 CB	61 CD2	90.78
130 N	129 CB	156 N	104.26	130 N	129 CB	61 CG	104.14
130 N	129 CB	131 OG	61.97	130 N	129 CB	131 N	33.82
130 N	129 CB	152 N	133.95	130 N	129 CB	130 CB	1.13
61 CE1	129 CB	152 SG	108.16	61 CE1	129 CB	300 OH2	137.92
61 CE1	129 CB	61 NE2	17.73	61 CE1	129 CB	128 CA	146.91
61 CE1	129 CB	61 ND1	12.53	61 CE1	129 CB	301 OH2	122.36
61 CE1	129 CB	130 CA	88.15	61 CE1	129 CB	130 C	73.82
61 CE1	129 CB	130 O	73.61	61 CE1	129 CB	152 CB	92.90
61 CE1	129 CB	128 N	153.80	61 CE1	129 CB	128 CB	143.90
61 CE1	129 CB	61 CD2	18.54	61 CE1	129 CB	156 N	112.06
61 CE1	129 CB	61 CG	14.21	61 CE1	129 CB	131 OG	36.42
61 CE1	129 CB	131 N	64.58	61 CE1	129 CB	152 N	103.95
61 CE1	129 CB	130 CB	97.20	152 SG	129 CB	300 OH2	94.36

Fig. 11X

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
152 SG	129 CB	61 NE2	118.86	152 SG	129 CB	128 CA	66.76
152 SG	129 CB	61 ND1	95.64	152 SG	129 CB	301 OH2	126.29
152 SG	129 CB	130 CA	157.27	152 SG	129 CB	130 C	173.08
152 SG	129 CB	130 O	172.92	152 SG	129 CB	152 CB	16.65
152 SG	129 CB	128 N	55.90	152 SG	129 CB	128 CB	82.22
152 SG	129 CB	61 CD2	110.60	152 SG	129 CB	156 N	77.22
152 SG	129 CB	61 CG	99.17	152 SG	129 CB	131 OG	142.57
152 SG	129 CB	131 N	164.52	152 SG	129 CB	152 N	27.47
152 SG	129 CB	130 CB	151.94	300 OH2	129 CB	61 NE2	141.32
300 OH2	129 CB	128 CA	74.53	300 OH2	129 CB	61 ND1	143.09
300 OH2	129 CB	301 OH2	35.18	300 OH2	129 CB	130 CA	82.90
300 OH2	129 CB	130 C	88.09	300 OH2	129 CB	130 O	80.29
300 OH2	129 CB	152 CB	110.64	300 OH2	129 CB	128 N	67.80
300 OH2	129 CB	128 CB	72.49	300 OH2	129 CB	61 CD2	150.21
300 OH2	129 CB	156 N	38.42	300 OH2	129 CB	61 CG	151.89
300 OH2	129 CB	131 OG	120.40	300 OH2	129 CB	131 N	99.85
300 OH2	129 CB	152 N	111.55	300 OH2	129 CB	130 CB	73.52
61 NE2	129 CB	128 CA	134.62	61 NE2	129 CB	61 ND1	27.20
61 NE2	129 CB	301 OH2	114.70	61 NE2	129 CB	130 CA	73.54
61 NE2	129 CB	130 C	61.38	61 NE2	129 CB	130 O	64.72
61 NE2	129 CB	152 CB	102.39	61 NE2	129 CB	128 N	146.72
61 NE2	129 CB	128 CB	127.67	61 NE2	129 CB	61 CD2	9.04
61 NE2	129 CB	156 N	126.43	61 NE2	129 CB	61 CG	20.07
61 NE2	129 CB	131 OG	23.71	61 NE2	129 CB	131 N	50.70
61 NE2	129 CB	152 N	106.83	61 NE2	129 CB	130 CB	83.15
128 CA	129 CB	61 ND1	141.54	128 CA	129 CB	301 OH2	79.00
128 CA	129 CB	130 CA	90.88	128 CA	129 CB	130 C	107.82
128 CA	129 CB	130 O	115.68	128 CA	129 CB	152 CB	75.88
128 CA	129 CB	128 N	14.93	128 CA	129 CB	128 CB	15.46

Fig. 11Y

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 CA	129 CB	61 CD2	129.64	128 CA	129 CB	156 N	98.95
128 CA	129 CB	61 CG	133.53	128 CA	129 CB	131 OG	132.09
128 CA	129 CB	131 N	111.16	128 CA	129 CB	152 N	55.63
128 CA	129 CB	130 CB	85.45	61 ND1	129 CB	301 OH2	134.25
61 ND1	129 CB	130 CA	100.04	61 ND1	129 CB	130 C	86.20
61 ND1	129 CB	130 O	86.09	61 ND1	129 CB	152 CB	80.41
61 ND1	129 CB	128 N	144.00	61 ND1	129 CB	128 CB	144.13
61 ND1	129 CB	61 CD2	23.75	61 ND1	129 CB	156 N	110.53
61 ND1	129 CB	61 CG	11.33	61 ND1	129 CB	131 OG	48.47
61 ND1	129 CB	131 N	76.61	61 ND1	129 CB	152 N	92.64
61 ND1	129 CB	130 CB	109.32	301 OH2	129 CB	130 CA	47.72
301 OH2	129 CB	130 C	54.55	301 OH2	129 CB	130 O	50.06
301 OH2	129 CB	152 CB	142.88	301 OH2	129 CB	128 N	81.17
301 OH2	129 CB	128 CB	68.22	301 OH2	129 CB	61 CD2	123.10
301 OH2	129 CB	156 N	68.45	301 OH2	129 CB	61 CG	133.81
301 OH2	129 CB	131 OG	91.04	301 OH2	129 CB	131 N	66.16
301 OH2	129 CB	152 N	132.86	301 OH2	129 CB	130 CB	38.41
130 CA	129 CB	130 C	16.95	130 CA	129 CB	130 O	27.17
130 CA	129 CB	152 CB	157.06	130 CA	129 CB	128 N	102.82
130 CA	129 CB	128 CB	75.43	130 CA	129 CB	61 CD2	79.96
130 CA	129 CB	156 N	111.90	130 CA	129 CB	61 CG	93.38
130 CA	129 CB	131 OG	51.74	130 CA	129 CB	131 N	23.61
130 CA	129 CB	152 N	134.48	130 CA	129 CB	130 CB	9.87
130 C	129 CB	130 O	13.56	130 C	129 CB	152 CB	161.05
130 C	129 CB	128 N	119.60	130 C	129 CB	128 CB	92.38
130 C	129 CB	61 CD2	69.08	130 C	129 CB	156 N	108.42
130 C	129 CB	61 CG	81.40	130 C	129 CB	131 OG	38.01
130 C	129 CB	131 N	11.76	130 C	129 CB	152 N	145.96
130 C	129 CB	130 CB	23.95	130 O	129 CB	152 CB	166.51

Fig. 11Z

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 O	129 CB	128 N	125.03	130 O	129 CB	128 CB	100.40
130 O	129 CB	61 CD2	73.34	130 O	129 CB	156 N	95.74
130 O	129 CB	61 CG	83.84	130 O	129 CB	131 OG	41.22
130 O	129 CB	131 N	22.34	130 O	129 CB	152 N	159.50
130 O	129 CB	130 CB	30.39	152 CB	129 CB	128 N	67.82
152 CB	129 CB	128 CB	90.71	152 CB	129 CB	61 CD2	94.01
152 CB	129 CB	156 N	88.92	152 CB	129 CB	61 CG	82.95
152 CB	129 CB	131 OG	126.08	152 CB	129 CB	131 N	149.40
152 CB	129 CB	152 N	23.91	152 CB	129 CB	130 CB	158.54
128 N	129 CB	128 CB	28.64	128 N	129 CB	61 CD2	139.98
128 N	129 CB	156 N	86.12	128 N	129 CB	61 CG	139.61
128 N	129 CB	131 OG	147.02	128 N	129 CB	131 N	124.62
128 N	129 CB	152 N	51.70	128 N	129 CB	130 CB	96.07
128 CB	129 CB	61 CD2	125.36	128 CB	129 CB	156 N	103.91
128 CB	129 CB	61 CG	133.60	128 CB	129 CB	131 OG	119.22
128 CB	129 CB	131 N	96.16	128 CB	129 CB	152 N	69.20
128 CB	129 CB	130 CB	70.09	61 CD2	129 CB	156 N	130.54
61 CD2	129 CB	61 CG	13.87	61 CD2	129 CB	131 OG	32.14
61 CD2	129 CB	131 N	57.95	61 CD2	129 CB	152 N	97.80
61 CD2	129 CB	130 CB	89.76	156 N	129 CB	61 CG	121.76
156 N	129 CB	131 OG	120.78	156 N	129 CB	131 N	117.94
156 N	129 CB	152 N	103.82	156 N	129 CB	130 CB	104.59
61 CG	129 CB	131 OG	43.51	61 CG	129 CB	131 N	70.76
61 CG	129 CB	152 N	90.92	61 CG	129 CB	130 CB	103.09
131 OG	129 CB	131 N	28.17	131 OG	129 CB	152 N	127.54
131 OG	129 CB	130 CB	60.85	131 N	129 CB	152 N	138.10
131 N	129 CB	130 CB	32.71	152 N	129 CB	130 CB	134.62
61 CE1	129 OG	130 N	113.14	61 CE1	129 OG	61 NE2	20.27
61 CE1	129 OG	61 ND1	12.36	61 CE1	129 OG	130 O	93.42

Fig. 11AA

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CE1	129 OG	300 OH2	176.66	61 CE1	129 OG	128 C	130.71
61 CE1	129 OG	128 O	145.08	61 CE1	129 OG	130 C	89.02
61 CE1	129 OG	130 CA	100.37	61 CE1	129 OG	301 OH2	147.01
61 CE1	129 OG	131 OG	45.19	61 CE1	129 OG	61 CD2	16.07
61 CE1	129 OG	152 SG	101.09	61 CE1	129 OG	61 CG	7.75
61 CE1	129 OG	131 N	76.12	61 CE1	129 OG	156 N	136.70
61 CE1	129 OG	157 NH2	117.58	61 CE1	129 OG	128 CA	123.12
61 CE1	129 OG	156 CG	109.17	61 CE1	129 OG	131 CA	68.19
61 CE1	129 OG	130 CB	109.12	130 N	129 OG	61 NE2	92.95
130 N	129 OG	61 ND1	124.41	130 N	129 OG	130 O	40.07
130 N	129 OG	300 OH2	69.38	130 N	129 OG	128 C	62.86
130 N	129 OG	128 O	67.46	130 N	129 OG	130 C	31.85
130 N	129 OG	130 CA	14.20	130 N	129 OG	301 OH2	37.58
130 N	129 OG	131 OG	72.37	130 N	129 OG	61 CD2	98.29
130 N	129 OG	152 SG	115.76	130 N	129 OG	61 CG	113.45
130 N	129 OG	131 N	41.26	130 N	129 OG	156 N	107.78
130 N	129 OG	157 NH2	45.83	130 N	129 OG	128 CA	65.22
130 N	129 OG	156 CG	125.75	130 N	129 OG	131 CA	53.93
130 N	129 OG	130 CB	10.29	61 NE2	129 OG	61 ND1	31.69
61 NE2	129 OG	130 O	78.24	61 NE2	129 OG	300 OH2	162.32
61 NE2	129 OG	128 C	120.93	61 NE2	129 OG	128 O	136.74
61 NE2	129 OG	130 C	70.99	61 NE2	129 OG	130 CA	80.51
61 NE2	129 OG	301 OH2	128.29	61 NE2	129 OG	131 OG	29.73
61 NE2	129 OG	61 CD2	7.04	61 NE2	129 OG	152 SG	110.27
61 NE2	129 OG	61 CG	21.48	61 NE2	129 OG	131 N	57.82
61 NE2	129 OG	156 N	155.80	61 NE2	129 OG	157 NH2	105.24
61 NE2	129 OG	128 CA	114.23	61 NE2	129 OG	156 CG	126.34
61 NE2	129 OG	131 CA	52.46	61 NE2	129 OG	130 CB	89.53
61 ND1	129 OG	130 O	105.44	61 ND1	129 OG	300 OH2	165.87

Fig. 11BB

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 ND1	129 OG	128 C	128.28	61 ND1	129 OG	128 O	140.06
61 ND1	129 OG	130 C	101.38	61 ND1	129 OG	130 CA	112.20
61 ND1	129 OG	301 OH2	159.37	61 ND1	129 OG	131 OG	57.52
61 ND1	129 OG	61 CD2	26.13	61 ND1	129 OG	152 SG	90.64
61 ND1	129 OG	61 CG	11.21	61 ND1	129 OG	131 N	88.45
61 ND1	129 OG	156 N	127.16	61 ND1	129 OG	157 NH2	128.31
61 ND1	129 OG	128 CA	120.69	61 ND1	129 OG	156 CG	102.28
61 ND1	129 OG	131 CA	80.44	61 ND1	129 OG	130 CB	121.15
130 O	129 OG	300 OH2	87.31	130 O	129 OG	128 C	102.28
130 O	129 OG	128 O	103.40	130 O	129 OG	130 C	15.35
130 O	129 OG	130 CA	30.16	130 O	129 OG	301 OH2	54.68
130 O	129 OG	131 OG	48.86	130 O	129 OG	61 CD2	85.27
130 O	129 OG	152 SG	155.79	130 O	129 OG	61 CG	98.37
130 O	129 OG	131 N	24.48	130 O	129 OG	156 N	109.59
130 O	129 OG	157 NH2	27.96	130 O	129 OG	128 CA	105.24
130 O	129 OG	156 CG	106.81	130 O	129 OG	131 CA	25.80
130 O	129 OG	130 CB	29.80	300 OH2	129 OG	128 C	52.14
300 OH2	129 OG	128 O	37.46	300 OH2	129 OG	130 C	92.51
300 OH2	129 OG	130 CA	81.88	300 OH2	129 OG	301 OH2	34.58
300 OH2	129 OG	131 OG	135.94	300 OH2	129 OG	61 CD2	167.07
300 OH2	129 OG	152 SG	79.33	300 OH2	129 OG	61 CG	173.70
300 OH2	129 OG	131 N	105.53	300 OH2	129 OG	156 N	40.19
300 OH2	129 OG	157 NH2	62.35	300 OH2	129 OG	128 CA	59.69
300 OH2	129 OG	156 CG	67.52	300 OH2	129 OG	131 CA	112.81
300 OH2	129 OG	130 CB	72.97	128 C	129 OG	128 O	15.81
128 C	129 OG	130 C	94.21	128 C	129 OG	130 CA	75.58
128 C	129 OG	301 OH2	59.62	128 C	129 OG	131 OG	123.97
128 C	129 OG	61 CD2	119.43	128 C	129 OG	152 SG	53.66
128 C	129 OG	61 CG	123.41	128 C	129 OG	131 N	100.46

Fig. 11CC

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 C	129 OG	156 N	80.68	128 C	129 OG	157 NH2	94.32
128 C	129 OG	128 CA	7.65	128 C	129 OG	156 CG	110.24
128 C	129 OG	131 CA	114.32	128 C	129 OG	130 CB	72.85
128 O	129 OG	130 C	99.16	128 O	129 OG	130 CA	81.41
128 O	129 OG	301 OH2	52.90	128 O	129 OG	131 OG	136.12
128 O	129 OG	61 CD2	135.08	128 O	129 OG	152 SG	54.48
128 O	129 OG	61 CG	137.44	128 O	129 OG	131 N	108.16
128 O	129 OG	156 N	65.26	128 O	129 OG	157 NH2	88.50
128 O	129 OG	128 CA	22.79	128 O	129 OG	156 CG	95.10
128 O	129 OG	131 CA	121.34	128 O	129 OG	130 CB	76.37
130 C	129 OG	130 CA	18.65	130 C	129 OG	301 OH2	57.99
130 C	129 OG	131 OG	44.14	130 C	129 OG	61 CD2	77.74
130 C	129 OG	152 SG	144.58	130 C	129 OG	61 CG	92.33
130 C	129 OG	131 N	13.18	130 C	129 OG	156 N	121.63
130 C	129 OG	157 NH2	40.20	130 C	129 OG	128 CA	95.54
130 C	129 OG	156 CG	122.10	130 C	129 OG	131 CA	22.69
130 C	129 OG	130 CB	22.92	130 CA	129 OG	301 OH2	48.23
130 CA	129 OG	131 OG	58.29	130 CA	129 OG	61 CD2	86.40
130 CA	129 OG	152 SG	126.71	130 CA	129 OG	61 CG	101.68
130 CA	129 OG	131 N	27.06	130 CA	129 OG	156 N	118.10
130 CA	129 OG	157 NH2	45.01	130 CA	129 OG	128 CA	76.95
130 CA	129 OG	156 CG	129.72	130 CA	129 OG	131 CA	39.94
130 CA	129 OG	130 CB	9.44	301 OH2	129 OG	131 OG	101.90
301 OH2	129 OG	61 CD2	134.52	301 OH2	129 OG	152 SG	106.62
301 OH2	129 OG	61 CG	149.73	301 OH2	129 OG	131 N	70.96
301 OH2	129 OG	156 N	70.36	301 OH2	129 OG	157 NH2	35.63
301 OH2	129 OG	128 CA	66.25	301 OH2	129 OG	156 CG	90.18
301 OH2	129 OG	131 CA	79.12	301 OH2	129 OG	130 CB	38.96
131 OG	129 OG	61 CD2	36.75	131 OG	129 OG	152 SG	138.48

Fig. 11DD

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
131 OG	129 OG	61 CG	49.56	131 OG	129 OG	131 N	31.80
131 OG	129 OG	156 N	147.23	131 OG	129 OG	157 NH2	75.51
131 OG	129 OG	128 CA	120.50	131 OG	129 OG	156 CG	123.03
131 OG	129 OG	131 CA	23.15	131 OG	129 OG	130 CB	65.81
61 CD2	129 OG	152 SG	103.66	61 CD2	129 OG	61 CG	15.28
61 CD2	129 OG	131 N	64.55	61 CD2	129 OG	156 N	152.74
61 CD2	129 OG	157 NH2	112.26	61 CD2	129 OG	128 CA	112.30
61 CD2	129 OG	156 CG	124.89	61 CD2	129 OG	131 CA	59.49
61 CD2	129 OG	130 CB	95.58	152 SG	129 OG	61 CG	94.40
152 SG	129 OG	131 N	143.85	152 SG	129 OG	156 N	72.30
152 SG	129 OG	157 NH2	141.06	152 SG	129 OG	128 CA	50.56
152 SG	129 OG	156 CG	86.71	152 SG	129 OG	131 CA	153.82
152 SG	129 OG	130 CB	126.01	61 CG	129 OG	131 N	79.20
61 CG	129 OG	156 N	138.35	61 CG	129 OG	157 NH2	123.80
61 CG	129 OG	128 CA	115.78	61 CG	129 OG	156 CG	113.00
61 CG	129 OG	131 CA	72.71	61 CG	129 OG	130 CB	110.83
131 N	129 OG	156 N	133.82	131 N	129 OG	157 NH2	51.90
131 N	129 OG	128 CA	100.18	131 N	129 OG	156 CG	128.70
131 N	129 OG	131 CA	13.88	131 N	129 OG	130 CB	34.03
156 N	129 OG	157 NH2	81.92	156 N	129 OG	128 CA	86.42
156 N	129 OG	156 CG	29.98	156 N	129 OG	131 CA	132.20
156 N	129 OG	130 CB	108.66	157 NH2	129 OG	128 CA	100.22
157 NH2	129 OG	156 CG	84.94	157 NH2	129 OG	131 CA	53.12
157 NH2	129 OG	130 CB	38.10	128 CA	129 OG	156 CG	115.36
128 CA	129 OG	131 CA	114.01	128 CA	129 OG	130 CB	75.45
156 CG	129 OG	131 CA	119.15	156 CG	129 OG	130 CB	121.60
131 CA	129 OG	130 CB	45.55	61 CE1	129 P1	156 N	160.22
61 CE1	129 P1	300 OH2	139.22	61 CE1	129 P1	156 CG	131.59
61 CE1	129 P1	156 CB	148.07	61 CE1	129 P1	130 N	80.66

Fig. 11EE

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CE1	129 P1	61 ND1	13.22	61 CE1	129 P1	61 NE2	13.08
61 CE1	129 P1	301 OH2	115.69	61 CE1	129 P1	128 O	108.39
61 CE1	129 P1	156 CA	162.21	61 CE1	129 P1	130 O	75.79
61 CE1	129 P1	128 C	95.20	61 CE1	129 P1	156 NE	115.09
61 CE1	129 P1	156 CD	120.41	61 CE1	129 P1	152 SG	85.51
61 CE1	129 P1	130 C	68.87	61 CE1	129 P1	157 N	171.54
61 CE1	129 P1	157 NH2	104.68	61 CE1	129 P1	130 CA	74.65
61 CE1	129 P1	131 OG	35.42	61 CE1	129 P1	156 C	171.97
61 CE1	129 P1	61 CD2	6.38	61 CE1	129 P1	61 CG	6.75
156 N	129 P1	300 OH2	50.28	156 N	129 P1	156 CG	41.20
156 N	129 P1	156 CB	32.96	156 N	129 P1	130 N	113.58
156 N	129 P1	61 ND1	147.71	156 N	129 P1	61 NE2	169.99
156 N	129 P1	301 OH2	80.11	156 N	129 P1	128 O	71.99
156 N	129 P1	156 CA	15.51	156 N	129 P1	130 O	123.79
156 N	129 P1	128 C	84.89	156 N	129 P1	156 NE	65.19
156 N	129 P1	156 CD	54.54	156 N	129 P1	152 SG	79.90
156 N	129 P1	130 C	129.77	156 N	129 P1	157 N	27.92
156 N	129 P1	157 NH2	95.08	156 N	129 P1	130 CA	121.58
156 N	129 P1	131 OG	164.33	156 N	129 P1	156 C	21.78
156 N	129 P1	61 CD2	165.23	156 N	129 P1	61 CG	153.74
300 OH2	129 P1	156 CG	88.69	300 OH2	129 P1	156 CB	72.59
300 OH2	129 P1	130 N	63.63	300 OH2	129 P1	61 ND1	147.11
300 OH2	129 P1	61 NE2	129.07	300 OH2	129 P1	301 OH2	33.82
300 OH2	129 P1	128 O	35.39	300 OH2	129 P1	156 CA	57.64
300 OH2	129 P1	130 O	84.24	300 OH2	129 P1	128 C	47.18
300 OH2	129 P1	156 NE	104.41	300 OH2	129 P1	156 CD	100.36
300 OH2	129 P1	152 SG	78.74	300 OH2	129 P1	130 C	84.51
300 OH2	129 P1	157 N	36.07	300 OH2	129 P1	157 NH2	64.64
300 OH2	129 P1	130 CA	72.75	300 OH2	129 P1	131 OG	120.30

Fig. 11FF

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
300 OH2	129 P1	156 C	48.25	300 OH2	129 P1	61 CD2	134.07
300 OH2	129 P1	61 CG	143.08	156 CG	129 P1	156 CB	19.77
156 CG	129 P1	130 N	144.26	156 CG	129 P1	61 ND1	120.48
156 CG	129 P1	61 NE2	142.11	156 CG	129 P1	301 OH2	110.10
156 CG	129 P1	128 O	112.89	156 CG	129 P1	156 CA	31.05
156 CG	129 P1	130 O	127.40	156 CG	129 P1	128 C	125.34
156 CG	129 P1	156 NE	27.40	156 CG	129 P1	156 CD	13.55
156 CG	129 P1	152 SG	102.02	156 CG	129 P1	130 C	139.37
156 CG	129 P1	157 N	55.01	156 CG	129 P1	157 NH2	102.99
156 CG	129 P1	130 CA	144.93	156 CG	129 P1	131 OG	138.24
156 CG	129 P1	156 C	41.95	156 CG	129 P1	61 CD2	137.18
156 CG	129 P1	61 CG	126.35	156 CB	129 P1	130 N	124.51
156 CB	129 P1	61 ND1	138.88	156 CB	129 P1	61 NE2	154.67
156 CB	129 P1	301 OH2	90.51	156 CB	129 P1	128 O	102.50
156 CB	129 P1	156 CA	17.99	156 CB	129 P1	130 O	112.83
156 CB	129 P1	128 C	115.77	156 CB	129 P1	156 NE	33.62
156 CB	129 P1	156 CD	28.17	156 CB	129 P1	152 SG	108.97
156 CB	129 P1	130 C	123.99	156 CB	129 P1	157 N	37.02
156 CB	129 P1	157 NH2	85.57	156 CB	129 P1	130 CA	126.15
156 CB	129 P1	131 OG	138.57	156 CB	129 P1	156 C	24.35
156 CB	129 P1	61 CD2	152.28	156 CB	129 P1	61 CG	144.10
130 N	129 P1	61 ND1	93.23	130 N	129 P1	61 NE2	68.06
130 N	129 P1	301 OH2	35.15	130 N	129 P1	128 O	56.58
130 N	129 P1	156 CA	116.98	130 N	129 P1	130 O	34.31
130 N	129 P1	128 C	50.42	130 N	129 P1	156 NE	135.42
130 N	129 P1	156 CD	147.20	130 N	129 P1	152 SG	94.56
130 N	129 P1	130 C	26.26	130 N	129 P1	157 N	91.57
130 N	129 P1	157 NH2	46.05	130 N	129 P1	130 CA	11.07
130 N	129 P1	131 OG	57.22	130 N	129 P1	156 C	104.25

Fig. 11GG

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 N	129 P1	61 CD2	74.38	130 N	129 P1	61 CG	86.87
61 ND1	129 P1	61 NE2	26.30	61 ND1	129 P1	301 OH2	128.39
61 ND1	129 P1	128 O	112.81	61 ND1	129 P1	156 CA	149.74
61 ND1	129 P1	130 O	88.49	61 ND1	129 P1	128 C	100.28
61 ND1	129 P1	156 NE	108.42	61 ND1	129 P1	156 CD	110.72
61 ND1	129 P1	152 SG	80.36	61 ND1	129 P1	130 C	82.02
61 ND1	129 P1	157 N	175.14	61 ND1	129 P1	157 NH2	116.92
61 ND1	129 P1	130 CA	87.73	61 ND1	129 P1	131 OG	47.60
61 ND1	129 P1	156 C	162.35	61 ND1	129 P1	61 CD2	19.55
61 ND1	129 P1	61 CG	6.53	61 NE2	129 P1	301 OH2	102.88
61 NE2	129 P1	128 O	102.52	61 NE2	129 P1	156 CA	172.55
61 NE2	129 P1	130 O	63.53	61 NE2	129 P1	128 C	89.31
61 NE2	129 P1	156 NE	121.23	61 NE2	129 P1	156 CD	129.64
61 NE2	129 P1	152 SG	90.16	61 NE2	129 P1	130 C	55.98
61 NE2	129 P1	157 N	158.51	61 NE2	129 P1	157 NH2	92.73
61 NE2	129 P1	130 CA	61.64	61 NE2	129 P1	131 OG	24.73
61 NE2	129 P1	156 C	167.68	61 NE2	129 P1	61 CD2	6.76
61 NE2	129 P1	61 CG	19.79	301 OH2	129 P1	128 O	49.34
301 OH2	129 P1	156 CA	81.85	301 OH2	129 P1	130 O	50.46
301 OH2	129 P1	128 C	53.22	301 OH2	129 P1	156 NE	111.93
301 OH2	129 P1	156 CD	116.98	301 OH2	129 P1	152 SG	99.48
301 OH2	129 P1	130 C	51.22	301 OH2	129 P1	157 N	56.42
301 OH2	129 P1	157 NH2	35.96	301 OH2	129 P1	130 CA	41.53
301 OH2	129 P1	131 OG	87.77	301 OH2	129 P1	156 C	69.12
301 OH2	129 P1	61 CD2	109.36	301 OH2	129 P1	61 CG	121.99
128 O	129 P1	156 CA	84.93	128 O	129 P1	130 O	89.58
128 O	129 P1	128 C	13.28	128 O	129 P1	156 NE	136.12
128 O	129 P1	156 CD	126.41	128 O	129 P1	152 SG	50.23
128 O	129 P1	130 C	82.84	128 O	129 P1	157 N	69.40

Fig. 11HH

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 O	129 P1	157 NH2	85.06	128 O	129 P1	130 CA	67.62
128 O	129 P1	131 OG	107.36	128 O	129 P1	156 C	79.64
128 O	129 P1	61 CD2	105.11	128 O	129 P1	61 CG	110.19
156 CA	129 P1	130 O	117.05	156 CA	129 P1	128 C	98.15
156 CA	129 P1	156 NE	51.33	156 CA	129 P1	156 CD	43.15
156 CA	129 P1	152 SG	94.77	156 CA	129 P1	130 C	125.91
156 CA	129 P1	157 N	25.43	156 CA	129 P1	157 NH2	87.81
156 CA	129 P1	130 CA	122.31	156 CA	129 P1	131 OG	152.46
156 CA	129 P1	156 C	13.29	156 CA	129 P1	61 CD2	168.17
156 CA	129 P1	61 CG	156.15	130 O	129 P1	128 C	84.69
130 O	129 P1	156 NE	106.06	130 O	129 P1	156 CD	121.37
130 O	129 P1	152 SG	127.11	130 O	129 P1	130 C	12.04
130 O	129 P1	157 N	95.90	130 O	129 P1	157 NH2	29.29
130 O	129 P1	130 CA	24.39	130 O	129 P1	131 OG	41.06
130 O	129 P1	156 C	104.57	130 O	129 P1	61 CD2	70.02
130 O	129 P1	61 CG	82.42	128 C	129 P1	156 NE	149.39
128 C	129 P1	156 CD	138.89	128 C	129 P1	152 SG	47.87
128 C	129 P1	130 C	76.02	128 C	129 P1	157 N	82.23
128 C	129 P1	157 NH2	86.83	128 C	129 P1	130 CA	60.96
128 C	129 P1	131 OG	95.83	128 C	129 P1	156 C	92.82
128 C	129 P1	61 CD2	91.83	128 C	129 P1	61 CG	97.26
156 NE	129 P1	156 CD	15.91	156 NE	129 P1	152 SG	126.59
156 NE	129 P1	130 C	117.71	156 NE	129 P1	157 N	68.39
156 NE	129 P1	157 NH2	89.47	156 NE	129 P1	130 CA	129.22
156 NE	129 P1	131 OG	111.20	156 NE	129 P1	156 C	56.96
156 NE	129 P1	61 CD2	118.74	156 NE	129 P1	61 CG	112.34
156 CD	129 P1	152 SG	110.86	156 CD	129 P1	130 C	133.22
156 CD	129 P1	157 N	65.17	156 CD	129 P1	157 NH2	101.71
156 CD	129 P1	130 CA	143.37	156 CD	129 P1	131 OG	124.95

Fig. 11III

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CD	129 P1	156 C	52.36	156 CD	129 P1	61 CD2	125.43
156 CD	129 P1	61 CG	115.98	152 SG	129 P1	130 C	115.68
152 SG	129 P1	157 N	98.52	152 SG	129 P1	157 NH2	134.57
152 SG	129 P1	130 CA	103.08	152 SG	129 P1	131 OG	112.13
152 SG	129 P1	156 C	100.27	152 SG	129 P1	61 CD2	87.21
152 SG	129 P1	61 CG	82.29	130 C	129 P1	157 N	102.67
130 C	129 P1	157 NH2	38.81	130 C	129 P1	130 CA	15.24
130 C	129 P1	131 OG	36.68	130 C	129 P1	156 C	112.86
130 C	129 P1	61 CD2	62.70	130 C	129 P1	61 CG	75.62
157 N	129 P1	157 NH2	67.21	157 N	129 P1	130 CA	97.13
157 N	129 P1	131 OG	136.58	157 N	129 P1	156 C	13.06
157 N	129 P1	61 CD2	165.26	157 N	129 P1	61 CG	178.29
157 NH2	129 P1	130 CA	42.28	157 NH2	129 P1	131 OG	69.37
157 NH2	129 P1	156 C	75.29	157 NH2	129 P1	61 CD2	99.12
157 NH2	129 P1	61 CG	111.15	130 CA	129 P1	131 OG	47.57
130 CA	129 P1	156 C	109.09	130 CA	129 P1	61 CD2	68.27
130 CA	129 P1	61 CG	81.21	131 OG	129 P1	156 C	142.99
131 OG	129 P1	61 CD2	30.35	131 OG	129 P1	61 CG	41.79
156 C	129 P1	61 CD2	172.50	156 C	129 P1	61 CG	168.26
61 CD2	129 P1	61 CG	13.04	156 CG	129 O3	156 N	44.94
156 CG	129 O3	61 CE1	139.30	156 CG	129 O3	156 CB	18.96
156 CG	129 O3	152 SG	127.31	156 CG	129 O3	61 ND1	138.22
156 CG	129 O3	156 CD	15.17	156 CG	129 O3	156 CA	31.17
156 CG	129 O3	300 OH2	83.24	156 CG	129 O3	156 NE	26.79
156 CG	129 O3	61 NE2	139.77	156 CG	129 O3	128 O	111.24
156 CG	129 O3	152 CB	132.32	156 CG	129 O3	128 C	123.04
156 CG	129 O3	61 CG	140.34	156 N	129 O3	61 CE1	151.94
156 N	129 O3	156 CB	33.19	156 N	129 O3	152 SG	91.89
156 N	129 O3	61 ND1	168.38	156 N	129 O3	156 CD	60.05

Fig. 11JJ

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 N	129 O3	156 CA	14.97	156 N	129 O3	300 OH2	44.24
156 N	129 O3	156 NE	67.31	156 N	129 O3	61 NE2	144.55
156 N	129 O3	128 O	67.05	156 N	129 O3	152 CB	105.96
156 N	129 O3	128 C	78.99	156 N	129 O3	61 CG	166.21
61 CE1	129 O3	156 CB	137.50	61 CE1	129 O3	152 SG	93.33
61 CE1	129 O3	61 ND1	16.45	61 CE1	129 O3	156 CD	126.40
61 CE1	129 O3	156 CA	149.44	61 CE1	129 O3	300 OH2	110.12
61 CE1	129 O3	156 NE	112.52	61 CE1	129 O3	61 NE2	7.61
61 CE1	129 O3	128 O	95.57	61 CE1	129 O3	152 CB	85.59
61 CE1	129 O3	128 C	84.56	61 CE1	129 O3	61 CG	14.39
156 CB	129 O3	152 SG	124.45	156 CB	129 O3	61 ND1	144.61
156 CB	129 O3	156 CD	31.06	156 CB	129 O3	156 CA	18.30
156 CB	129 O3	300 OH2	65.25	156 CB	129 O3	156 NE	34.39
156 CB	129 O3	61 NE2	134.37	156 CB	129 O3	128 O	94.96
156 CB	129 O3	152 CB	136.12	156 CB	129 O3	128 C	106.26
156 CB	129 O3	61 CG	145.58	152 SG	129 O3	61 ND1	90.69
152 SG	129 O3	156 CD	138.18	152 SG	129 O3	156 CA	106.35
152 SG	129 O3	300 OH2	79.03	152 SG	129 O3	156 NE	153.86
152 SG	129 O3	61 NE2	92.64	152 SG	129 O3	128 O	50.74
152 SG	129 O3	152 CB	17.66	152 SG	129 O3	128 C	47.01
152 SG	129 O3	61 CG	89.37	61 ND1	129 O3	156 CD	123.27
61 ND1	129 O3	156 CA	161.45	61 ND1	129 O3	300 OH2	125.51
61 ND1	129 O3	156 NE	112.92	61 ND1	129 O3	61 NE2	23.91
61 ND1	129 O3	128 O	106.37	61 ND1	129 O3	152 CB	78.93
61 ND1	129 O3	128 C	94.60	61 ND1	129 O3	61 CG	2.75
156 CD	129 O3	156 CA	45.96	156 CD	129 O3	300 OH2	96.27
156 CD	129 O3	156 NE	16.37	156 CD	129 O3	61 NE2	128.52
156 CD	129 O3	128 O	125.70	156 CD	129 O3	152 CB	137.84
156 CD	129 O3	128 C	137.24	156 CD	129 O3	61 CG	125.50

Fig. 11KK

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CA	129 O3	300 OH2	53.48	156 CA	129 O3	156 NE	52.34
156 CA	129 O3	61 NE2	143.76	156 CA	129 O3	128 O	80.08
156 CA	129 O3	152 CB	119.32	156 CA	129 O3	128 C	91.92
156 CA	129 O3	61 CG	161.54	300 OH2	129 O3	156 NE	94.88
300 OH2	129 O3	61 NE2	102.55	300 OH2	129 O3	128 O	31.42
300 OH2	129 O3	152 CB	96.59	300 OH2	129 O3	128 C	41.52
300 OH2	129 O3	61 CG	122.87	156 NE	129 O3	61 NE2	113.49
156 NE	129 O3	128 O	126.27	156 NE	129 O3	152 CB	153.58
156 NE	129 O3	128 C	135.82	156 NE	129 O3	61 CG	114.68
61 NE2	129 O3	128 O	89.27	61 NE2	129 O3	152 CB	87.07
61 NE2	129 O3	128 C	78.66	61 NE2	129 O3	61 CG	21.67
128 O	129 O3	152 CB	67.40	128 O	129 O3	128 C	11.94
128 O	129 O3	61 CG	103.68	152 CB	129 O3	128 C	61.88
152 CB	129 O3	61 CG	78.21	128 C	129 O3	61 CG	91.94
61 CE1	129 O4	156 CG	132.12	61 CE1	129 O4	156 NE	137.68
61 CE1	129 O4	156 CB	148.60	61 CE1	129 O4	130 O	81.80
61 CE1	129 O4	61 NE2	14.19	61 CE1	129 O4	61 ND1	13.26
61 CE1	129 O4	156 CD	131.53	61 CE1	129 O4	156 N	125.39
61 CE1	129 O4	130 N	74.49	61 CE1	129 O4	300 OH2	110.23
61 CE1	129 O4	157 NH2	113.37	61 CE1	129 O4	131 OG	41.87
61 CE1	129 O4	130 C	71.79	61 CE1	129 O4	156 CA	140.25
61 CE1	129 O4	301 OH2	104.47	61 CE1	129 O4	156 CZ	138.05
61 CE1	129 O4	156 NH2	136.64	61 CE1	129 O4	61 CD2	10.66
61 CE1	129 O4	130 CA	72.61	61 CE1	129 O4	61 CG	9.64
61 CE1	129 O4	131 N	63.15	61 CE1	129 O4	131 CA	64.24
156 CG	129 O4	156 NE	32.73	156 CG	129 O4	156 CB	19.87
156 CG	129 O4	130 O	143.15	156 CG	129 O4	61 NE2	146.23
156 CG	129 O4	61 ND1	120.94	156 CG	129 O4	156 CD	17.40
156 CG	129 O4	156 N	36.83	156 CG	129 O4	130 N	129.68

Fig. 11LL

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CG	129 O4	300 OH2	76.26	156 CG	129 O4	157 NH2	111.29
156 CG	129 O4	131 OG	170.23	156 CG	129 O4	130 C	149.87
156 CG	129 O4	156 CA	27.93	156 CG	129 O4	301 OH2	101.11
156 CG	129 O4	156 CZ	41.85	156 CG	129 O4	156 NH2	55.16
156 CG	129 O4	61 CD2	141.46	156 CG	129 O4	130 CA	140.37
156 CG	129 O4	61 CG	128.56	156 CG	129 O4	131 N	161.36
156 CG	129 O4	131 CA	163.48	156 NE	129 O4	156 CB	38.31
156 NE	129 O4	130 O	133.07	156 NE	129 O4	61 NE2	147.28
156 NE	129 O4	61 ND1	124.62	156 NE	129 O4	156 CD	17.31
156 NE	129 O4	156 N	66.64	156 NE	129 O4	130 N	147.68
156 NE	129 O4	300 OH2	101.37	156 NE	129 O4	157 NH2	105.79
156 NE	129 O4	131 OG	142.56	156 NE	129 O4	130 C	144.30
156 NE	129 O4	156 CA	52.91	156 NE	129 O4	301 OH2	116.66
156 NE	129 O4	156 CZ	9.39	156 NE	129 O4	156 NH2	23.15
156 NE	129 O4	61 CD2	139.81	156 NE	129 O4	130 CA	148.64
156 NE	129 O4	61 CG	128.88	156 NE	129 O4	131 N	146.78
156 NE	129 O4	131 CA	135.96	156 CB	129 O4	130 O	123.28
156 CB	129 O4	61 NE2	160.92	156 CB	129 O4	61 ND1	139.39
156 CB	129 O4	156 CD	30.75	156 CB	129 O4	156 N	30.14
156 CB	129 O4	130 N	114.70	156 CB	129 O4	300 OH2	63.37
156 CB	129 O4	157 NH2	91.51	156 CB	129 O4	131 OG	168.78
156 CB	129 O4	130 C	130.50	156 CB	129 O4	156 CA	14.87
156 CB	129 O4	301 OH2	83.94	156 CB	129 O4	156 CZ	45.01
156 CB	129 O4	156 NH2	55.34	156 CB	129 O4	61 CD2	159.09
156 CB	129 O4	130 CA	123.10	156 CB	129 O4	61 CG	147.30
156 CB	129 O4	131 N	141.68	156 CB	129 O4	131 CA	145.51
130 O	129 O4	61 NE2	67.89	130 O	129 O4	61 ND1	94.34
130 O	129 O4	156 CD	146.08	130 O	129 O4	156 N	116.38
130 O	129 O4	130 N	33.74	130 O	129 O4	300 OH2	78.21

Fig. 11MM

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 O	129 O4	157 NH2	32.14	130 O	129 O4	131 OG	46.10
130 O	129 O4	130 C	11.23	130 O	129 O4	156 CA	117.93
130 O	129 O4	301 OH2	48.80	130 O	129 O4	156 CZ	125.63
130 O	129 O4	156 NH2	113.52	130 O	129 O4	61 CD2	74.05
130 O	129 O4	130 CA	21.60	130 O	129 O4	61 CG	87.27
130 O	129 O4	131 N	18.90	130 O	129 O4	131 CA	25.27
61 NE2	129 O4	61 ND1	26.48	61 NE2	129 O4	156 CD	144.80
61 NE2	129 O4	156 N	133.13	61 NE2	129 O4	130 N	64.73
61 NE2	129 O4	300 OH2	108.43	61 NE2	129 O4	157 NH2	99.78
61 NE2	129 O4	131 OG	28.47	61 NE2	129 O4	130 C	58.24
61 NE2	129 O4	156 CA	149.03	61 NE2	129 O4	301 OH2	96.03
61 NE2	129 O4	156 CZ	144.58	61 NE2	129 O4	156 NH2	138.38
61 NE2	129 O4	61 CD2	7.52	61 NE2	129 O4	130 CA	60.67
61 NE2	129 O4	61 CG	19.98	61 NE2	129 O4	131 N	49.12
61 NE2	129 O4	131 CA	50.21	61 ND1	129 O4	156 CD	118.52
61 ND1	129 O4	156 N	122.62	61 ND1	129 O4	130 N	87.34
61 ND1	129 O4	300 OH2	117.38	61 ND1	129 O4	157 NH2	126.25
61 ND1	129 O4	131 OG	51.74	61 ND1	129 O4	130 C	84.68
61 ND1	129 O4	156 CA	135.18	61 ND1	129 O4	301 OH2	116.44
61 ND1	129 O4	156 CZ	125.79	61 ND1	129 O4	156 NH2	126.63
61 ND1	129 O4	61 CD2	20.54	61 ND1	129 O4	130 CA	85.87
61 ND1	129 O4	61 CG	7.97	61 ND1	129 O4	131 N	75.50
61 ND1	129 O4	131 CA	74.89	156 CD	129 O4	156 N	53.98
156 CD	129 O4	130 N	145.31	156 CD	129 O4	300 OH2	92.55
156 CD	129 O4	157 NH2	115.09	156 CD	129 O4	131 OG	154.98
156 CD	129 O4	130 C	156.62	156 CD	129 O4	156 CA	43.08
156 CD	129 O4	301 OH2	114.65	156 CD	129 O4	156 CZ	26.67
156 CD	129 O4	156 NH2	40.45	156 CD	129 O4	61 CD2	137.82
156 CD	129 O4	130 CA	153.42	156 CD	129 O4	61 CG	124.83

Fig. 11NN

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CD	129 O4	131 N	163.04	156 CD	129 O4	131 CA	153.27
156 N	129 O4	130 N	93.33	156 N	129 O4	300 OH2	40.15
156 N	129 O4	157 NH2	91.84	156 N	129 O4	131 OG	150.56
156 N	129 O4	130 C	117.60	156 N	129 O4	156 CA	15.94
156 N	129 O4	301 OH2	67.99	156 N	129 O4	156 CZ	74.42
156 N	129 O4	156 NH2	85.44	156 N	129 O4	61 CD2	135.25
156 N	129 O4	130 CA	105.18	156 N	129 O4	61 CG	129.62
156 N	129 O4	131 N	128.60	156 N	129 O4	131 CA	141.03
130 N	129 O4	300 OH2	53.44	130 N	129 O4	157 NH2	47.30
130 N	129 O4	131 OG	59.26	130 N	129 O4	130 C	27.34
130 N	129 O4	156 CA	102.39	130 N	129 O4	301 OH2	31.53
130 N	129 O4	156 CZ	146.38	130 N	129 O4	156 NH2	139.84
130 N	129 O4	61 CD2	72.25	130 N	129 O4	130 CA	13.20
130 N	129 O4	61 CG	83.44	130 N	129 O4	131 N	36.12
130 N	129 O4	131 CA	50.15	300 OH2	129 O4	157 NH2	62.62
300 OH2	129 O4	131 OG	112.42	300 OH2	129 O4	130 C	77.71
300 OH2	129 O4	156 CA	49.58	300 OH2	129 O4	301 OH2	29.69
300 OH2	129 O4	156 CZ	106.55	300 OH2	129 O4	156 NH2	112.53
300 OH2	129 O4	61 CD2	114.72	300 OH2	129 O4	130 CA	65.04
300 OH2	129 O4	61 CG	119.35	300 OH2	129 O4	131 N	88.49
300 OH2	129 O4	131 CA	101.43	157 NH2	129 O4	131 OG	77.53
157 NH2	129 O4	130 C	41.59	157 NH2	129 O4	156 CA	88.51
157 NH2	129 O4	301 OH2	36.39	157 NH2	129 O4	156 CZ	100.95
157 NH2	129 O4	156 NH2	92.57	157 NH2	129 O4	61 CD2	106.14
157 NH2	129 O4	130 CA	42.97	157 NH2	129 O4	61 CG	119.37
157 NH2	129 O4	131 N	51.04	157 NH2	129 O4	131 CA	54.89
131 OG	129 O4	130 C	39.89	131 OG	129 O4	156 CA	161.57
131 OG	129 O4	301 OH2	88.51	131 OG	129 O4	156 CZ	134.24
131 OG	129 O4	156 NH2	121.97	131 OG	129 O4	61 CD2	31.69

Fig. 1100

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
131 OG	129 O4	130 CA	49.15	131 OG	129 O4	61 CG	43.87
131 OG	129 O4	131 N	28.33	131 OG	129 O4	131 CA	23.27
130 C	129 O4	156 CA	122.51	130 C	129 O4	301 OH2	49.95
130 C	129 O4	156 CZ	136.72	130 C	129 O4	156 NH2	124.28
130 C	129 O4	61 CD2	64.86	130 C	129 O4	130 CA	14.14
130 C	129 O4	61 CG	78.04	130 C	129 O4	131 N	11.67
130 C	129 O4	131 CA	23.76	156 CA	129 O4	301 OH2	73.18
156 CA	129 O4	156 CZ	59.86	156 CA	129 O4	156 NH2	70.03
156 CA	129 O4	61 CD2	150.57	156 CA	129 O4	130 CA	112.47
156 CA	129 O4	61 CG	142.84	156 CA	129 O4	131 N	134.17
156 CA	129 O4	131 CA	142.94	301 OH2	129 O4	156 CZ	117.48
301 OH2	129 O4	156 NH2	116.13	301 OH2	129 O4	61 CD2	103.52
301 OH2	129 O4	130 CA	39.40	301 OH2	129 O4	61 CG	113.87
301 OH2	129 O4	131 N	61.43	301 OH2	129 O4	131 CA	73.05
156 CZ	129 O4	156 NH2	13.78	156 CZ	129 O4	61 CD2	137.58
156 CZ	129 O4	130 CA	143.67	156 CZ	129 O4	61 CG	128.59
156 CZ	129 O4	131 N	137.83	156 CZ	129 O4	131 CA	126.60
156 NH2	129 O4	61 CD2	132.66	156 NH2	129 O4	130 CA	133.42
156 NH2	129 O4	61 CG	127.09	156 NH2	129 O4	131 N	124.26
156 NH2	129 O4	131 CA	112.82	61 CD2	129 O4	130 CA	68.00
61 CD2	129 O4	61 CG	13.22	61 CD2	129 O4	131 N	55.15
61 CD2	129 O4	131 CA	54.56	130 CA	129 O4	61 CG	80.49
130 CA	129 O4	131 N	23.54	130 CA	129 O4	131 CA	37.24
61 CG	129 O4	131 N	68.36	61 CG	129 O4	131 CA	67.07
131 N	129 O4	131 CA	14.24	300 OH2	129 O5	156 N	73.74
300 OH2	129 O5	156 CB	100.13	300 OH2	129 O5	301 OH2	44.20
300 OH2	129 O5	156 CA	80.43	300 OH2	129 O5	156 CG	116.78
300 OH2	129 O5	128 O	42.55	300 OH2	129 O5	157 N	51.91
300 OH2	129 O5	130 N	75.33	300 OH2	129 O5	156 C	66.97

Fig. 11PP

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
300 OH2	129 O5	128 C	53.95	300 OH2	129 O5	130 O	97.63
300 OH2	129 O5	157 NH2	79.96	300 OH2	129 O5	61 CE1	136.71
300 OH2	129 O5	157 CB	42.13	300 OH2	129 O5	156 CD	125.03
300 OH2	129 O5	157 CG	57.07	300 OH2	129 O5	156 NE	129.74
300 OH2	129 O5	157 CA	45.83	300 OH2	129 O5	152 SG	87.51
300 OH2	129 O5	157 NE	61.51	300 OH2	129 O5	130 CA	81.60
300 OH2	129 O5	130 C	94.55	300 OH2	129 O5	156 O	70.21
300 OH2	129 O5	157 CZ	73.74	300 OH2	129 O5	61 NE2	128.70
156 N	129 O5	156 CB	39.52	156 N	129 O5	301 OH2	112.43
156 N	129 O5	156 CA	19.45	156 N	129 O5	156 CG	45.47
156 N	129 O5	128 O	93.63	156 N	129 O5	157 N	40.99
156 N	129 O5	130 N	149.06	156 N	129 O5	156 C	30.96
156 N	129 O5	128 C	105.71	156 N	129 O5	130 O	153.38
156 N	129 O5	157 NH2	122.43	156 N	129 O5	61 CE1	138.61
156 N	129 O5	157 CB	67.31	156 N	129 O5	156 CD	55.74
156 N	129 O5	157 CG	75.53	156 N	129 O5	156 NE	68.19
156 N	129 O5	157 CA	51.07	156 N	129 O5	152 SG	85.59
156 N	129 O5	157 NE	101.00	156 N	129 O5	130 CA	154.34
156 N	129 O5	130 C	161.23	156 N	129 O5	156 O	33.97
156 N	129 O5	157 CZ	110.79	156 N	129 O5	61 NE2	149.55
156 CB	129 O5	301 OH2	118.47	156 CB	129 O5	156 CA	22.53
156 CB	129 O5	156 CG	21.64	156 CB	129 O5	128 O	132.06
156 CB	129 O5	157 N	49.09	156 CB	129 O5	130 N	150.25
156 CB	129 O5	156 C	33.24	156 CB	129 O5	128 C	144.89
156 CB	129 O5	130 O	121.94	156 CB	129 O5	157 NH2	100.01
156 CB	129 O5	61 CE1	123.05	156 CB	129 O5	157 CB	69.94
156 CB	129 O5	156 CD	25.66	156 CB	129 O5	157 CG	66.53
156 CB	129 O5	156 NE	31.49	156 CB	129 O5	157 CA	57.62
156 CB	129 O5	152 SG	115.90	156 CB	129 O5	157 NE	88.66

Fig. 11QQ

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CB	129 O5	130 CA	143.54	156 CB	129 O5	130 C	133.13
156 CB	129 O5	156 O	30.46	156 CB	129 O5	157 CZ	91.23
156 CB	129 O5	61 NE2	130.83	301 OH2	129 O5	156 CA	109.76
301 OH2	129 O5	156 CG	139.98	301 OH2	129 O5	128 O	60.85
301 OH2	129 O5	157 N	75.70	301 OH2	129 O5	130 N	39.59
301 OH2	129 O5	156 C	91.36	301 OH2	129 O5	128 C	62.16
301 OH2	129 O5	130 O	53.54	301 OH2	129 O5	157 NH2	40.50
301 OH2	129 O5	61 CE1	107.94	301 OH2	129 O5	157 CB	50.16
301 OH2	129 O5	156 CD	139.36	301 OH2	129 O5	157 CG	52.09
301 OH2	129 O5	156 NE	129.06	301 OH2	129 O5	157 CA	65.32
301 OH2	129 O5	152 SG	110.63	301 OH2	129 O5	157 NE	34.33
301 OH2	129 O5	130 CA	42.05	301 OH2	129 O5	130 C	52.00
301 OH2	129 O5	156 O	91.90	301 OH2	129 O5	157 CZ	40.02
301 OH2	129 O5	61 NE2	96.96	156 CA	129 O5	156 CG	36.53
156 CA	129 O5	128 O	109.55	156 CA	129 O5	157 N	34.12
156 CA	129 O5	130 N	149.21	156 CA	129 O5	156 C	18.59
156 CA	129 O5	128 C	122.54	156 CA	129 O5	130 O	135.95
156 CA	129 O5	157 NH2	107.15	156 CA	129 O5	61 CE1	140.69
156 CA	129 O5	157 CB	59.93	156 CA	129 O5	156 CD	44.78
156 CA	129 O5	157 CG	63.28	156 CA	129 O5	156 NE	53.73
156 CA	129 O5	157 CA	44.44	156 CA	129 O5	152 SG	104.23
156 CA	129 O5	157 NE	88.79	156 CA	129 O5	130 CA	148.53
156 CA	129 O5	130 C	146.20	156 CA	129 O5	156 O	19.20
156 CA	129 O5	157 CZ	96.11	156 CA	129 O5	61 NE2	150.57
156 CG	129 O5	128 O	135.81	156 CG	129 O5	157 N	68.82
156 CG	129 O5	130 N	161.15	156 CG	129 O5	156 C	52.47
156 CG	129 O5	128 C	144.27	156 CG	129 O5	130 O	127.52
156 CG	129 O5	157 NH2	115.08	156 CG	129 O5	61 CE1	104.57
156 CG	129 O5	157 CB	91.39	156 CG	129 O5	156 CD	10.66

Fig. 11RR

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CG	129 O5	157 CG	87.90	156 CG	129 O5	156 NE	25.64
156 CG	129 O5	157 CA	78.19	156 CG	129 O5	152 SG	101.15
156 CG	129 O5	157 NE	108.51	156 CG	129 O5	130 CA	152.00
156 CG	129 O5	130 C	137.26	156 CG	129 O5	156 O	50.63
156 CG	129 O5	157 CZ	108.56	156 CG	129 O5	61 NE2	114.05
128 O	129 O5	157 N	91.41	128 O	129 O5	130 N	62.99
128 O	129 O5	156 C	103.41	128 O	129 O5	128 C	13.44
128 O	129 O5	130 O	96.46	128 O	129 O5	157 NH2	100.16
128 O	129 O5	61 CE1	98.11	128 O	129 O5	157 CB	84.40
128 O	129 O5	156 CD	146.23	128 O	129 O5	157 CG	98.09
128 O	129 O5	156 NE	161.28	128 O	129 O5	157 CA	87.50
128 O	129 O5	152 SG	51.22	128 O	129 O5	157 NE	93.02
128 O	129 O5	130 CA	72.12	128 O	129 O5	130 C	86.92
128 O	129 O5	156 O	107.60	128 O	129 O5	157 CZ	100.84
128 O	129 O5	61 NE2	93.91	157 N	129 O5	130 N	115.28
157 N	129 O5	156 C	16.35	157 N	129 O5	128 C	104.36
157 N	129 O5	130 O	114.00	157 N	129 O5	157 NH2	82.75
157 N	129 O5	61 CE1	170.41	157 N	129 O5	157 CB	26.68
157 N	129 O5	156 CD	74.72	157 N	129 O5	157 CG	35.40
157 N	129 O5	156 NE	77.85	157 N	129 O5	157 CA	10.51
157 N	129 O5	152 SG	115.63	157 N	129 O5	157 NE	60.23
157 N	129 O5	130 CA	116.29	157 N	129 O5	130 C	120.26
157 N	129 O5	156 O	18.63	157 N	129 O5	157 CZ	71.08
157 N	129 O5	61 NE2	167.38	130 N	129 O5	156 C	130.64
130 N	129 O5	128 C	54.31	130 N	129 O5	130 O	33.64
130 N	129 O5	157 NH2	50.30	130 N	129 O5	61 CE1	68.67
130 N	129 O5	157 CB	89.28	130 N	129 O5	156 CD	150.75
130 N	129 O5	157 CG	87.43	130 N	129 O5	156 NE	135.51
130 N	129 O5	157 CA	104.85	130 N	129 O5	152 SG	93.48

Fig. 11SS

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 N	129 O5	157 NE	63.06	130 N	129 O5	130 CA	9.14
130 N	129 O5	130 C	24.04	130 N	129 O5	156 O	130.61
130 N	129 O5	157 CZ	59.12	130 N	129 O5	61 NE2	57.87
156 C	129 O5	128 C	116.81	156 C	129 O5	130 O	122.42
156 C	129 O5	157 NH2	91.59	156 C	129 O5	61 CE1	156.28
156 C	129 O5	157 CB	41.37	156 C	129 O5	156 CD	58.71
156 C	129 O5	157 CG	45.57	156 C	129 O5	156 NE	63.41
156 C	129 O5	157 CA	26.20	156 C	129 O5	152 SG	114.75
156 C	129 O5	157 NE	71.29	156 C	129 O5	130 CA	130.32
156 C	129 O5	130 C	130.96	156 C	129 O5	156 O	4.55
156 C	129 O5	157 CZ	80.05	156 C	129 O5	61 NE2	162.69
128 C	129 O5	130 O	87.81	128 C	129 O5	157 NH2	97.97
128 C	129 O5	61 CE1	85.07	128 C	129 O5	157 CB	94.55
128 C	129 O5	156 CD	153.35	128 C	129 O5	157 CG	106.50
128 C	129 O5	156 NE	168.29	128 C	129 O5	157 CA	99.66
128 C	129 O5	152 SG	48.53	128 C	129 O5	157 NE	96.26
128 C	129 O5	130 CA	63.36	128 C	129 O5	130 C	77.41
128 C	129 O5	156 O	120.96	128 C	129 O5	157 CZ	101.39
128 C	129 O5	61 NE2	80.49	130 O	129 O5	157 NH2	31.33
130 O	129 O5	61 CE1	63.91	130 O	129 O5	157 CB	89.21
130 O	129 O5	156 CD	117.30	130 O	129 O5	157 CG	78.69
130 O	129 O5	156 NE	101.90	130 O	129 O5	157 CA	104.77
130 O	129 O5	152 SG	119.71	130 O	129 O5	157 NE	53.99
130 O	129 O5	130 CA	24.50	130 O	129 O5	130 C	11.20
130 O	129 O5	156 O	119.46	130 O	129 O5	157 CZ	43.03
130 O	129 O5	61 NE2	54.02	157 NH2	129 O5	61 CE1	94.35
157 NH2	129 O5	157 CB	59.02	157 NH2	129 O5	156 CD	108.18
157 NH2	129 O5	157 CG	47.38	157 NH2	129 O5	156 NE	93.71
157 NH2	129 O5	157 CA	73.88	157 NH2	129 O5	152 SG	143.56

Fig. 11TT

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
157 NH2	129 O5	157 NE	23.57	157 NH2	129 O5	130 CA	44.01
157 NH2	129 O5	130 C	39.47	157 NH2	129 O5	156 O	89.07
157 NH2	129 O5	157 CZ	11.70	157 NH2	129 O5	61 NE2	85.05
61 CE1	129 O5	157 CB	153.12	61 CE1	129 O5	156 CD	97.67
61 CE1	129 O5	157 CG	140.55	61 CE1	129 O5	156 NE	93.27
61 CE1	129 O5	157 CA	167.75	61 CE1	129 O5	152 SG	71.87
61 CE1	129 O5	157 NE	117.72	61 CE1	129 O5	130 CA	66.10
61 CE1	129 O5	130 C	59.49	61 CE1	129 O5	156 O	153.05
61 CE1	129 O5	157 CZ	105.72	61 CE1	129 O5	61 NE2	11.05
157 CB	129 O5	156 CD	94.57	157 CB	129 O5	157 CG	16.44
157 CB	129 O5	156 NE	92.15	157 CB	129 O5	157 CA	16.28
157 CB	129 O5	152 SG	126.72	157 CB	129 O5	157 NE	35.50
157 CB	129 O5	130 CA	89.66	157 CB	129 O5	130 C	94.12
157 CB	129 O5	156 O	41.75	157 CB	129 O5	157 CZ	47.93
157 CB	129 O5	61 NE2	142.86	156 CD	129 O5	157 CG	88.22
156 CD	129 O5	156 NE	15.61	156 CD	129 O5	157 CA	83.20
156 CD	129 O5	152 SG	107.03	156 CD	129 O5	157 NE	105.61
156 CD	129 O5	130 CA	141.64	156 CD	129 O5	130 C	126.74
156 CD	129 O5	156 O	56.11	156 CD	129 O5	157 CZ	103.31
156 CD	129 O5	61 NE2	106.27	157 CG	129 O5	156 NE	82.09
157 CG	129 O5	157 CA	27.23	157 CG	129 O5	152 SG	143.13
157 CG	129 O5	157 NE	25.72	157 CG	129 O5	130 CA	85.26
157 CG	129 O5	130 C	85.81	157 CG	129 O5	156 O	44.10
157 CG	129 O5	157 CZ	35.69	157 CG	129 O5	61 NE2	132.23
156 NE	129 O5	157 CA	84.33	156 NE	129 O5	152 SG	119.98
156 NE	129 O5	157 NE	94.78	156 NE	129 O5	130 CA	126.36
156 NE	129 O5	130 C	111.71	156 NE	129 O5	156 O	59.81
156 NE	129 O5	157 CZ	90.23	156 NE	129 O5	61 NE2	99.80
157 CA	129 O5	152 SG	119.67	157 CA	129 O5	157 NE	50.78

Fig. 11UU

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
157 CA	129 O5	130 CA	105.80	157 CA	129 O5	130 C	110.28
157 CA	129 O5	156 O	27.56	157 CA	129 O5	157 CZ	62.37
157 CA	129 O5	61 NE2	158.78	152 SG	129 O5	157 NE	144.17
152 SG	129 O5	130 CA	100.55	152 SG	129 O5	130 C	108.94
152 SG	129 O5	156 O	118.66	152 SG	129 O5	157 CZ	149.62
152 SG	129 O5	61 NE2	76.41	157 NE	129 O5	130 CA	59.89
157 NE	129 O5	130 C	60.25	157 NE	129 O5	156 O	69.68
157 NE	129 O5	157 CZ	13.22	157 NE	129 O5	61 NE2	108.00
130 CA	129 O5	130 C	15.09	130 CA	129 O5	156 O	129.34
130 CA	129 O5	157 CZ	53.93	130 CA	129 O5	61 NE2	55.06
130 C	129 O5	156 O	128.54	130 C	129 O5	157 CZ	50.92
130 C	129 O5	61 NE2	48.79	156 O	129 O5	157 CZ	77.69
156 O	129 O5	61 NE2	158.40	157 CZ	129 O5	61 NE2	96.65
61 CE1	129 C5	61 ND1	20.43	61 CE1	129 C5	156 CG	129.94
61 CE1	129 C5	152 SG	94.34	61 CE1	129 C5	61 NE2	2.93
61 CE1	129 C5	156 CD	127.42	61 CE1	129 C5	156 N	121.58
61 CE1	129 C5	61 CG	22.36	61 CE1	129 C5	152 CB	92.78
61 CE1	129 C5	156 CB	120.17	61 CE1	129 C5	156 NE	112.25
61 CE1	129 C5	61 CD2	9.81	61 CE1	129 C5	61 CB	35.28
61 CE1	129 C5	156 CA	124.14	61 ND1	129 C5	156 CG	144.44
61 ND1	129 C5	152 SG	97.61	61 ND1	129 C5	61 NE2	23.16
61 ND1	129 C5	156 CD	135.70	61 ND1	129 C5	156 N	141.93
61 ND1	129 C5	61 CG	2.23	61 ND1	129 C5	152 CB	89.25
61 ND1	129 C5	156 CB	137.80	61 ND1	129 C5	156 NE	121.09
61 ND1	129 C5	61 CD2	10.86	61 ND1	129 C5	61 CB	14.93
61 ND1	129 C5	156 CA	144.11	156 CG	129 C5	152 SG	107.69
156 CG	129 C5	61 NE2	128.42	156 CG	129 C5	156 CD	16.19
156 CG	129 C5	156 N	34.82	156 CG	129 C5	61 CG	146.49
156 CG	129 C5	152 CB	122.12	156 CG	129 C5	156 CB	13.29

Fig. 11VV

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CG	129 C5	156 NE	25.92	156 CG	129 C5	61 CD2	138.39
156 CG	129 C5	61 CB	152.84	156 CG	129 C5	156 CA	22.55
152 SG	129 C5	61 NE2	92.77	152 SG	129 C5	156 CD	122.85
152 SG	129 C5	156 N	75.27	152 SG	129 C5	61 CG	96.72
152 SG	129 C5	152 CB	19.87	152 SG	129 C5	156 CB	101.85
152 SG	129 C5	156 NE	132.56	152 SG	129 C5	61 CD2	94.41
152 SG	129 C5	61 CB	97.51	152 SG	129 C5	156 CA	87.58
61 NE2	129 C5	156 CD	126.88	61 NE2	129 C5	156 N	118.79
61 NE2	129 C5	61 CG	25.04	61 NE2	129 C5	152 CB	92.14
61 NE2	129 C5	156 CB	118.21	61 NE2	129 C5	156 NE	111.82
61 NE2	129 C5	61 CD2	12.40	61 NE2	129 C5	61 CB	37.94
61 NE2	129 C5	156 CA	121.65	156 CD	129 C5	156 N	51.01
156 CD	129 C5	61 CG	137.29	156 CD	129 C5	152 CB	134.84
156 CD	129 C5	156 CB	27.10	156 CD	129 C5	156 NE	15.25
156 CD	129 C5	61 CD2	133.47	156 CD	129 C5	61 CB	139.47
156 CD	129 C5	156 CA	38.64	156 N	129 C5	61 CG	143.67
156 N	129 C5	152 CB	92.97	156 N	129 C5	156 CB	26.59
156 N	129 C5	156 NE	57.43	156 N	129 C5	61 CD2	131.07
156 N	129 C5	61 CB	156.21	156 N	129 C5	156 CA	12.57
61 CG	129 C5	152 CB	87.78	61 CG	129 C5	156 CB	140.02
61 CG	129 C5	156 NE	122.84	61 CG	129 C5	61 CD2	12.66
61 CG	129 C5	61 CB	12.92	61 CG	129 C5	156 CA	146.24
152 CB	129 C5	156 CB	119.09	152 CB	129 C5	156 NE	148.04
152 CB	129 C5	61 CD2	89.55	152 CB	129 C5	61 CB	84.84
152 CB	129 C5	156 CA	104.70	156 CB	129 C5	156 NE	30.88
156 CB	129 C5	61 CD2	129.49	156 CB	129 C5	61 CB	150.33
156 CB	129 C5	156 CA	14.41	156 NE	129 C5	61 CD2	118.24
156 NE	129 C5	61 CB	127.06	156 NE	129 C5	156 CA	45.00
61 CD2	129 C5	61 CB	25.54	61 CD2	129 C5	156 CA	133.94

Fig. 11WW

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CB	129 C5	156 CA	158.86	156 CG	129 C6	156 CD	21.02
156 CG	129 C6	156 NE	31.00	156 CG	129 C6	61 ND1	129.40
156 CG	129 C6	61 CE1	114.32	156 CG	129 C6	156 CB	10.11
156 CG	129 C6	156 N	33.35	156 CG	129 C6	156 CA	19.12
156 CG	129 C6	152 SG	99.39	156 CG	129 C6	156 CZ	37.07
156 CD	129 C6	156 NE	17.37	156 CD	129 C6	61 ND1	132.80
156 CD	129 C6	61 CE1	120.65	156 CD	129 C6	156 CB	28.86
156 CD	129 C6	156 N	54.37	156 CD	129 C6	156 CA	40.14
156 CD	129 C6	152 SG	120.30	156 CD	129 C6	156 CZ	20.33
156 NE	129 C6	61 ND1	116.13	156 NE	129 C6	61 CE1	105.36
156 NE	129 C6	156 CB	34.06	156 NE	129 C6	156 N	61.34
156 NE	129 C6	156 CA	48.12	156 NE	129 C6	152 SG	126.14
156 NE	129 C6	156 CZ	7.08	61 ND1	129 C6	61 CE1	15.51
61 ND1	129 C6	156 CB	120.13	61 ND1	129 C6	156 N	113.41
61 ND1	129 C6	156 CA	121.62	61 ND1	129 C6	152 SG	74.35
61 ND1	129 C6	156 CZ	115.90	61 CE1	129 C6	156 CB	104.82
61 CE1	129 C6	156 N	98.74	61 CE1	129 C6	156 CA	106.20
61 CE1	129 C6	152 SG	70.83	61 CE1	129 C6	156 CZ	106.70
156 CB	129 C6	156 N	27.32	156 CB	129 C6	156 CA	14.33
156 CB	129 C6	152 SG	93.16	156 CB	129 C6	156 CZ	40.92
156 N	129 C6	156 CA	14.24	156 N	129 C6	152 SG	66.21
156 N	129 C6	156 CZ	68.24	156 CA	129 C6	152 SG	80.34
156 CA	129 C6	156 CZ	54.81	152 SG	129 C6	156 CZ	133.22
152 SG	129 C7	61 ND1	118.21	152 SG	129 C7	152 CB	27.14
152 SG	129 C7	61 CE1	108.14	152 SG	129 C7	61 CG	114.67
152 SG	129 C7	61 NE2	103.13	152 SG	129 C7	152 CA	28.92
152 SG	129 C7	61 N	95.92	152 SG	129 C7	61 CB	118.12
152 SG	129 C7	156 CG	102.99	152 SG	129 C7	61 CD2	107.32
152 SG	129 C7	156 N	74.29	152 SG	129 C7	152 N	25.24

Fig. 11XX

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 ND1	129 C7	152 CB	114.46	61 ND1	129 C7	61 CE1	19.39
61 ND1	129 C7	61 CG	8.14	61 ND1	129 C7	61 NE2	20.53
61 ND1	129 C7	152 CA	112.84	61 ND1	129 C7	61 N	42.02
61 ND1	129 C7	61 CB	21.26	61 ND1	129 C7	156 CG	110.33
61 ND1	129 C7	61 CD2	11.04	61 ND1	129 C7	156 N	119.48
61 ND1	129 C7	152 N	103.06	152 CB	129 C7	61 CE1	113.88
152 CB	129 C7	61 CG	107.80	152 CB	129 C7	61 NE2	108.05
152 CB	129 C7	152 CA	2.13	152 CB	129 C7	61 N	78.98
152 CB	129 C7	61 CB	104.41	152 CB	129 C7	156 CG	125.54
152 CB	129 C7	61 CD2	105.81	152 CB	129 C7	156 N	99.13
152 CB	129 C7	152 N	13.89	61 CE1	129 C7	61 CG	25.26
61 CE1	129 C7	61 NE2	5.83	61 CE1	129 C7	152 CA	112.87
61 CE1	129 C7	61 N	55.62	61 CE1	129 C7	61 CB	39.89
61 CE1	129 C7	156 CG	98.69	61 CE1	129 C7	61 CD2	15.39
61 CE1	129 C7	156 N	101.61	61 CE1	129 C7	152 N	100.43
61 CG	129 C7	61 NE2	24.70	61 CG	129 C7	152 CA	106.06
61 CG	129 C7	61 N	33.88	61 CG	129 C7	61 CB	14.70
61 CG	129 C7	156 CG	118.44	61 CG	129 C7	61 CD2	11.97
61 CG	129 C7	156 N	126.67	61 CG	129 C7	152 N	97.19
61 NE2	129 C7	152 CA	107.03	61 NE2	129 C7	61 N	52.28
61 NE2	129 C7	61 CB	39.34	61 NE2	129 C7	156 CG	103.01
61 NE2	129 C7	61 CD2	13.25	61 NE2	129 C7	156 N	103.39
61 NE2	129 C7	152 N	94.63	152 CA	129 C7	61 N	76.95
152 CA	129 C7	61 CB	102.41	152 CA	129 C7	156 CG	127.67
152 CA	129 C7	61 CD2	104.38	152 CA	129 C7	156 N	101.23
152 CA	129 C7	152 N	13.57	61 N	129 C7	61 CB	25.61
61 N	129 C7	156 CG	152.22	61 N	129 C7	61 CD2	40.29
61 N	129 C7	156 N	151.82	61 N	129 C7	152 N	72.22
61 CB	129 C7	156 CG	127.37	61 CB	129 C7	61 CD2	26.30

Fig. 11YY

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CB	129 C7	156 N	140.71	61 CB	129 C7	152 N	96.45
156 CG	129 C7	61 CD2	113.43	156 CG	129 C7	156 N	29.41
156 CG	129 C7	152 N	128.23	61 CD2	129 C7	156 N	116.54
61 CD2	129 C7	152 N	93.59	156 N	129 C7	152 N	99.35
130 O	129 C8	157 NH2	42.10	130 O	129 C8	130 C	11.65
130 O	129 C8	61 CE1	89.41	130 O	129 C8	131 OG	54.82
130 O	129 C8	130 N	36.80	130 O	129 C8	61 NE2	75.02
130 O	129 C8	131 CA	31.85	130 O	129 C8	156 NE	158.00
130 O	129 C8	131 N	21.31	130 O	129 C8	157 CZ	53.05
130 O	129 C8	301 OH2	54.65	130 O	129 C8	156 CB	133.98
130 O	129 C8	130 CA	21.28	130 O	129 C8	156 CG	148.05
130 O	129 C8	131 CB	46.33	130 O	129 C8	61 ND1	98.41
130 O	129 C8	157 NH1	58.97	130 O	129 C8	300 OH2	82.99
130 O	129 C8	156 NH2	140.90	130 O	129 C8	157 NE	59.73
130 O	129 C8	156 CD	159.80	130 O	129 C8	156 N	118.33
130 O	129 C8	156 CZ	151.21	157 NH2	129 C8	130 C	52.25
157 NH2	129 C8	61 CE1	128.23	157 NH2	129 C8	131 OG	96.35
157 NH2	129 C8	130 N	55.55	157 NH2	129 C8	61 NE2	115.78
157 NH2	129 C8	131 CA	69.75	157 NH2	129 C8	156 NE	116.20
157 NH2	129 C8	131 N	63.34	157 NH2	129 C8	157 CZ	11.03
157 NH2	129 C8	301 OH2	40.53	157 NH2	129 C8	156 CB	96.69
157 NH2	129 C8	130 CA	50.93	157 NH2	129 C8	156 CG	113.40
157 NH2	129 C8	131 CB	85.78	157 NH2	129 C8	61 ND1	137.93
157 NH2	129 C8	157 NH1	21.27	157 NH2	129 C8	300 OH2	66.28
157 NH2	129 C8	156 NH2	106.87	157 NH2	129 C8	157 NE	19.85
157 NH2	129 C8	156 CD	119.35	157 NH2	129 C8	156 N	92.75
157 NH2	129 C8	156 CZ	112.15	130 C	129 C8	61 CE1	78.00
130 C	129 C8	131 OG	46.79	130 C	129 C8	130 N	31.15
130 C	129 C8	61 NE2	63.96	130 C	129 C8	131 CA	29.50

Fig. 11ZZ

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 C	129 C8	156 NE	168.13	130 C	129 C8	131 N	13.99
130 C	129 C8	157 CZ	63.28	130 C	129 C8	301 OH2	56.47
130 C	129 C8	156 CB	137.57	130 C	129 C8	130 CA	14.98
130 C	129 C8	156 CG	147.91	130 C	129 C8	131 CB	41.00
130 C	129 C8	61 ND1	87.16	130 C	129 C8	157 NH1	70.25
130 C	129 C8	300 OH2	82.27	130 C	129 C8	156 NH2	151.99
130 C	129 C8	157 NE	68.37	130 C	129 C8	156 CD	162.70
130 C	129 C8	156 N	117.45	130 C	129 C8	156 CZ	162.86
61 CE1	129 C8	131 OG	45.51	61 CE1	129 C8	130 N	74.89
61 CE1	129 C8	61 NE2	15.65	61 CE1	129 C8	131 CA	72.99
61 CE1	129 C8	156 NE	112.25	61 CE1	129 C8	131 N	70.44
61 CE1	129 C8	157 CZ	138.52	61 CE1	129 C8	301 OH2	102.92
61 CE1	129 C8	156 CB	114.75	61 CE1	129 C8	130 CA	77.29
61 CE1	129 C8	156 CG	100.97	61 CE1	129 C8	131 CB	59.43
61 CE1	129 C8	61 ND1	9.75	61 CE1	129 C8	157 NH1	148.17
61 CE1	129 C8	300 OH2	96.94	61 CE1	129 C8	156 NH2	124.87
61 CE1	129 C8	157 NE	136.13	61 CE1	129 C8	156 CD	103.95
61 CE1	129 C8	156 N	99.21	61 CE1	129 C8	156 CZ	118.76
131 OG	129 C8	130 N	66.23	131 OG	129 C8	61 NE2	30.53
131 OG	129 C8	131 CA	28.59	131 OG	129 C8	156 NE	144.90
131 OG	129 C8	131 N	33.64	131 OG	129 C8	157 CZ	106.91
131 OG	129 C8	301 OH2	99.37	131 OG	129 C8	156 CB	160.06
131 OG	129 C8	130 CA	56.23	131 OG	129 C8	156 CG	145.99
131 OG	129 C8	131 CB	13.92	131 OG	129 C8	61 ND1	50.99
131 OG	129 C8	157 NH1	108.79	131 OG	129 C8	300 OH2	115.99
131 OG	129 C8	156 NH2	135.83	131 OG	129 C8	157 NE	114.54
131 OG	129 C8	156 CD	144.28	131 OG	129 C8	156 N	138.94
131 OG	129 C8	156 CZ	142.41	130 N	129 C8	61 NE2	66.90
130 N	129 C8	131 CA	59.33	130 N	129 C8	156 NE	143.23

Fig. 11AAA

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 N	129 C8	131 N	42.27	130 N	129 C8	157 CZ	64.39
130 N	129 C8	301 OH2	33.85	130 N	129 C8	156 CB	109.84
130 N	129 C8	130 CA	16.28	130 N	129 C8	156 CG	117.08
130 N	129 C8	131 CB	66.65	130 N	129 C8	61 ND1	84.43
130 N	129 C8	157 NH1	76.80	130 N	129 C8	300 OH2	52.99
130 N	129 C8	156 NH2	156.53	130 N	129 C8	157 NE	61.69
130 N	129 C8	156 CD	132.12	130 N	129 C8	156 N	87.04
130 N	129 C8	156 CZ	150.73	61 NE2	129 C8	131 CA	57.40
61 NE2	129 C8	156 NE	126.93	61 NE2	129 C8	131 N	55.24
61 NE2	129 C8	157 CZ	126.69	61 NE2	129 C8	301 OH2	98.80
61 NE2	129 C8	156 CB	129.54	61 NE2	129 C8	130 CA	65.68
61 NE2	129 C8	156 CG	116.48	61 NE2	129 C8	131 CB	44.37
61 NE2	129 C8	61 ND1	23.52	61 NE2	129 C8	157 NH1	133.94
61 NE2	129 C8	300 OH2	100.90	61 NE2	129 C8	156 NH2	135.42
61 NE2	129 C8	157 NE	128.04	61 NE2	129 C8	156 CD	119.46
61 NE2	129 C8	156 N	111.26	61 NE2	129 C8	156 CZ	132.07
131 CA	129 C8	156 NE	157.03	131 CA	129 C8	131 N	17.10
131 CA	129 C8	157 CZ	79.62	131 CA	129 C8	301 OH2	85.52
131 CA	129 C8	156 CB	165.76	131 CA	129 C8	130 CA	43.98
131 CA	129 C8	156 CG	173.42	131 CA	129 C8	131 CB	16.11
131 CA	129 C8	61 ND1	79.36	131 CA	129 C8	157 NH1	80.25
131 CA	129 C8	300 OH2	111.67	131 CA	129 C8	156 NH2	133.90
131 CA	129 C8	157 NE	89.20	131 CA	129 C8	156 CD	167.65
131 CA	129 C8	156 N	146.37	131 CA	129 C8	156 CZ	146.76
156 NE	129 C8	131 N	173.82	156 NE	129 C8	157 CZ	105.18
156 NE	129 C8	301 OH2	113.70	156 NE	129 C8	156 CB	33.55
156 NE	129 C8	130 CA	157.34	156 NE	129 C8	156 CG	27.70
156 NE	129 C8	131 CB	149.15	156 NE	129 C8	61 ND1	103.47
156 NE	129 C8	157 NH1	99.13	156 NE	129 C8	300 OH2	90.31

Fig. 11BBB

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 NE	129 C8	156 NH2	24.54	156 NE	129 C8	157 NE	99.76
156 NE	129 C8	156 CD	13.61	156 NE	129 C8	156 N	56.46
156 NE	129 C8	156 CZ	11.22	131 N	129 C8	157 CZ	74.22
131 N	129 C8	301 OH2	70.28	131 N	129 C8	156 CB	151.23
131 N	129 C8	130 CA	27.31	131 N	129 C8	156 CG	158.45
131 N	129 C8	131 CB	27.01	131 N	129 C8	61 ND1	78.74
131 N	129 C8	157 NH1	78.89	131 N	129 C8	300 OH2	94.92
131 N	129 C8	156 NH2	149.38	131 N	129 C8	157 NE	80.94
131 N	129 C8	156 CD	172.37	131 N	129 C8	156 N	129.27
131 N	129 C8	156 CZ	162.70	157 CZ	129 C8	301 OH2	43.51
157 CZ	129 C8	156 CB	87.29	157 CZ	129 C8	130 CA	61.43
157 CZ	129 C8	156 CG	104.08	157 CZ	129 C8	131 CB	95.73
157 CZ	129 C8	61 ND1	148.27	157 CZ	129 C8	157 NH1	13.87
157 CZ	129 C8	300 OH2	65.01	157 CZ	129 C8	156 NH2	96.56
157 CZ	129 C8	157 NE	13.22	157 CZ	129 C8	156 CD	108.81
157 CZ	129 C8	156 N	86.68	157 CZ	129 C8	156 CZ	101.23
301 OH2	129 C8	156 CB	81.11	301 OH2	129 C8	130 CA	43.75
301 OH2	129 C8	156 CG	93.45	301 OH2	129 C8	131 CB	97.10
301 OH2	129 C8	61 ND1	111.21	301 OH2	129 C8	157 NH1	57.32
301 OH2	129 C8	300 OH2	29.60	301 OH2	129 C8	156 NH2	122.74
301 OH2	129 C8	157 NE	34.49	301 OH2	129 C8	156 CD	106.82
301 OH2	129 C8	156 N	63.95	301 OH2	129 C8	156 CZ	118.21
156 CB	129 C8	130 CA	124.00	156 CB	129 C8	156 CG	16.79
156 CB	129 C8	131 CB	173.50	156 CB	129 C8	61 ND1	110.05
156 CB	129 C8	157 NH1	88.39	156 CB	129 C8	300 OH2	56.85
156 CB	129 C8	156 NH2	52.83	156 CB	129 C8	157 NE	77.01
156 CB	129 C8	156 CD	26.07	156 CB	129 C8	156 N	25.21
156 CB	129 C8	156 CZ	41.65	130 CA	129 C8	156 CG	132.98
130 CA	129 C8	131 CB	53.51	130 CA	129 C8	61 ND1	87.00

Fig. 11CCC

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 CA	129 C8	157 NH1	71.49	130 CA	129 C8	300 OH2	67.70
130 CA	129 C8	156 NH2	157.72	130 CA	129 C8	157 NE	62.93
130 CA	129 C8	156 CD	147.93	130 CA	129 C8	156 N	102.62
130 CA	129 C8	156 CZ	160.73	156 CG	129 C8	131 CB	159.40
156 CG	129 C8	61 ND1	95.01	156 CG	129 C8	157 NH1	104.67
156 CG	129 C8	300 OH2	65.91	156 CG	129 C8	156 NH2	51.66
156 CG	129 C8	157 NE	93.64	156 CG	129 C8	156 CD	15.05
156 CG	129 C8	156 N	30.51	156 CG	129 C8	156 CZ	38.52
131 CB	129 C8	61 ND1	64.67	131 CB	129 C8	157 NH1	95.92
131 CB	129 C8	300 OH2	119.37	131 CB	129 C8	156 NH2	132.16
131 CB	129 C8	157 NE	105.06	131 CB	129 C8	156 CD	153.85
131 CB	129 C8	156 N	149.00	131 CB	129 C8	156 CZ	142.44
61 ND1	129 C8	157 NH1	157.38	61 ND1	129 C8	300 OH2	101.66
61 ND1	129 C8	156 NH2	115.13	61 ND1	129 C8	157 NE	145.17
61 ND1	129 C8	156 CD	96.19	61 ND1	129 C8	156 N	98.04
61 ND1	129 C8	156 CZ	109.38	157 NH1	129 C8	300 OH2	77.03
157 NH1	129 C8	156 NH2	86.24	157 NH1	129 C8	157 NE	24.80
157 NH1	129 C8	156 CD	105.72	157 NH1	129 C8	156 N	93.53
157 NH1	129 C8	156 CZ	93.07	300 OH2	129 C8	156 NH2	107.72
300 OH2	129 C8	157 NE	52.36	300 OH2	129 C8	156 CD	80.44
300 OH2	129 C8	156 N	35.47	300 OH2	129 C8	156 CZ	98.19
156 NH2	129 C8	157 NE	96.54	156 NH2	129 C8	156 CD	38.15
156 NH2	129 C8	156 N	77.83	156 NH2	129 C8	156 CZ	13.33
157 NE	129 C8	156 CD	100.67	157 NE	129 C8	156 N	73.82
157 NE	129 C8	156 CZ	98.22	156 CD	129 C8	156 N	45.31
156 CD	129 C8	156 CZ	24.83	156 N	129 C8	156 CZ	65.97
130 O	129 C9	131 OG	63.44	130 O	129 C9	61 CE1	91.36
130 O	129 C9	131 CA	39.69	130 O	129 C9	61 NE2	80.02
130 O	129 C9	131 CB	57.37	130 O	129 C9	130 C	13.01

Fig. 11DDD

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 O	129 C9	131 N	27.17	130 O	129 C9	157 NH2	33.54
130 O	129 C9	61 ND1	103.34	130 O	129 C9	61 CD2	87.71
130 O	129 C9	130 N	28.42	130 O	129 C9	131 C	41.65
130 O	129 C9	156 NE	124.91	130 O	129 C9	130 CA	16.74
130 O	129 C9	61 CG	99.84	130 O	129 C9	156 NH2	126.93
130 O	129 C9	157 CZ	41.80	131 OG	129 C9	61 CE1	53.20
131 OG	129 C9	131 CA	34.08	131 OG	129 C9	61 NE2	35.30
131 OG	129 C9	131 CB	17.70	131 OG	129 C9	130 C	51.09
131 OG	129 C9	131 N	36.67	131 OG	129 C9	157 NH2	96.85
131 OG	129 C9	61 ND1	58.46	131 OG	129 C9	61 CD2	34.37
131 OG	129 C9	130 N	64.60	131 OG	129 C9	131 C	43.54
131 OG	129 C9	156 NE	159.39	131 OG	129 C9	130 CA	55.73
131 OG	129 C9	61 CG	47.62	131 OG	129 C9	156 NH2	168.07
131 OG	129 C9	157 CZ	104.90	61 CE1	129 C9	131 CA	84.09
61 CE1	129 C9	61 NE2	17.97	61 CE1	129 C9	131 CB	70.90
61 CE1	129 C9	130 C	80.11	61 CE1	129 C9	131 N	76.13
61 CE1	129 C9	157 NH2	115.71	61 CE1	129 C9	61 ND1	12.36
61 CE1	129 C9	61 CD2	21.94	61 CE1	129 C9	130 N	69.31
61 CE1	129 C9	131 C	94.95	61 CE1	129 C9	156 NE	106.25
61 CE1	129 C9	130 CA	74.95	61 CE1	129 C9	61 CG	17.50
61 CE1	129 C9	156 NH2	126.68	61 CE1	129 C9	157 CZ	122.39
131 CA	129 C9	61 NE2	66.51	131 CA	129 C9	131 CB	20.08
131 CA	129 C9	130 C	32.45	131 CA	129 C9	131 N	17.97
131 CA	129 C9	157 NH2	68.79	131 CA	129 C9	61 ND1	91.57
131 CA	129 C9	61 CD2	68.01	131 CA	129 C9	130 N	57.47
131 CA	129 C9	131 C	11.13	131 CA	129 C9	156 NE	162.96
131 CA	129 C9	130 CA	42.66	131 CA	129 C9	61 CG	81.51
131 CA	129 C9	156 NH2	149.22	131 CA	129 C9	157 CZ	75.64
61 NE2	129 C9	131 CB	52.98	61 NE2	129 C9	130 C	67.54

Fig. 11EEE

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 NE2	129 C9	131 N	60.47	61 NE2	129 C9	157 NH2	109.79
61 NE2	129 C9	61 ND1	25.74	61 NE2	129 C9	61 CD2	10.80
61 NE2	129 C9	130 N	63.90	61 NE2	129 C9	131 C	77.20
61 NE2	129 C9	156 NE	124.21	61 NE2	129 C9	130 CA	65.02
61 NE2	129 C9	61 CG	19.87	61 NE2	129 C9	156 NH2	144.23
61 NE2	129 C9	157 CZ	117.77	131 CB	129 C9	130 C	47.29
131 CB	129 C9	131 N	31.00	131 CB	129 C9	157 NH2	88.47
131 CB	129 C9	61 ND1	75.76	131 CB	129 C9	61 CD2	51.59
131 CB	129 C9	130 N	67.99	131 CB	129 C9	131 C	27.27
131 CB	129 C9	156 NE	176.71	131 CB	129 C9	130 CA	55.35
131 CB	129 C9	61 CG	64.38	131 CB	129 C9	156 NH2	158.19
131 CB	129 C9	157 CZ	95.59	130 C	129 C9	131 N	16.29
130 C	129 C9	157 NH2	46.35	130 C	129 C9	61 ND1	91.70
130 C	129 C9	61 CD2	74.84	130 C	129 C9	130 N	26.26
130 C	129 C9	131 C	37.90	130 C	129 C9	156 NE	134.51
130 C	129 C9	130 CA	10.98	130 C	129 C9	61 CG	87.24
130 C	129 C9	156 NH2	139.69	130 C	129 C9	157 CZ	54.68
131 N	129 C9	157 NH2	60.24	131 N	129 C9	61 ND1	86.13
131 N	129 C9	61 CD2	65.42	131 N	129 C9	130 N	39.66
131 N	129 C9	131 C	26.54	131 N	129 C9	156 NE	150.77
131 N	129 C9	130 CA	25.27	131 N	129 C9	61 CG	78.82
131 N	129 C9	156 NH2	152.50	131 N	129 C9	157 CZ	68.23
157 NH2	129 C9	61 ND1	127.86	157 NH2	129 C9	61 CD2	119.09
157 NH2	129 C9	130 N	46.72	157 NH2	129 C9	131 C	65.83
157 NH2	129 C9	156 NE	94.33	157 NH2	129 C9	130 CA	45.42
157 NH2	129 C9	61 CG	129.16	157 NH2	129 C9	156 NH2	93.40
157 NH2	129 C9	157 CZ	8.40	61 ND1	129 C9	61 CD2	24.18
61 ND1	129 C9	130 N	81.64	61 ND1	129 C9	131 C	101.82
61 ND1	129 C9	156 NE	101.12	61 ND1	129 C9	130 CA	87.11

Fig. 11FFF

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 ND1	129 C9	61 CG	12.58	61 ND1	129 C9	156 NH2	118.84
61 ND1	129 C9	157 CZ	134.21	61 CD2	129 C9	130 N	74.08
61 CD2	129 C9	131 C	77.89	61 CD2	129 C9	156 NE	125.29
61 CD2	129 C9	130 CA	73.76	61 CD2	129 C9	61 CG	13.63
61 CD2	129 C9	156 NH2	141.43	61 CD2	129 C9	157 CZ	127.30
130 N	129 C9	131 C	64.08	130 N	129 C9	156 NE	112.83
130 N	129 C9	130 CA	15.29	130 N	129 C9	61 CG	82.63
130 N	129 C9	156 NH2	127.30	130 N	129 C9	157 CZ	54.20
131 C	129 C9	156 NE	156.02	131 C	129 C9	130 CA	48.81
131 C	129 C9	61 CG	91.14	131 C	129 C9	156 NH2	138.34
131 C	129 C9	157 CZ	71.61	156 NE	129 C9	130 CA	125.97
156 NE	129 C9	61 CG	112.42	156 NE	129 C9	156 NH2	23.45
156 NE	129 C9	157 CZ	87.33	130 CA	129 C9	61 CG	84.85
130 CA	129 C9	156 NH2	135.96	130 CA	129 C9	157 CZ	53.75
61 CG	129 C9	156 NH2	127.81	61 CG	129 C9	157 CZ	136.83
156 NH2	129 C9	157 CZ	85.13	157 NH2	129 C10	130 O	41.76
157 NH2	129 C10	156 NE	149.70	157 NH2	129 C10	157 CZ	16.24
157 NH2	129 C10	156 CB	115.22	157 NH2	129 C10	157 NH1	29.16
157 NH2	129 C10	156 NH2	141.40	157 NH2	129 C10	157 NE	25.73
157 NH2	129 C10	156 CZ	146.55	157 NH2	129 C10	156 CG	130.43
157 NH2	129 C10	130 C	46.05	157 NH2	129 C10	157 CG	53.51
157 NH2	129 C10	156 CD	143.84	157 NH2	129 C10	301 OH2	39.20
157 NH2	129 C10	156 CA	103.56	157 NH2	129 C10	130 N	48.13
157 NH2	129 C10	157 CD	39.12	157 NH2	129 C10	300 OH2	66.88
157 NH2	129 C10	156 N	99.96	157 NH2	129 C10	157 N	79.24
157 NH2	129 C10	131 CA	61.88	157 NH2	129 C10	61 CE1	103.08
157 NH2	129 C10	156 C	91.36	157 NH2	129 C10	131 OG	81.58
157 NH2	129 C10	131 N	54.26	157 NH2	129 C10	130 CA	42.43
130 O	129 C10	156 NE	162.23	130 O	129 C10	157 CZ	57.91

Fig. 11GGG

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 O	129 C10	156 CB	135.27	130 O	129 C10	157 NH1	66.76
130 O	129 C10	156 NH2	160.81	130 O	129 C10	157 NE	65.43
130 O	129 C10	156 CZ	171.31	130 O	129 C10	156 CG	136.94
130 O	129 C10	130 C	5.62	130 O	129 C10	157 CG	91.37
130 O	129 C10	156 CD	151.08	130 O	129 C10	301 OH2	51.85
130 O	129 C10	156 CA	122.88	130 O	129 C10	130 N	29.31
130 O	129 C10	157 CD	79.46	130 O	129 C10	300 OH2	76.46
130 O	129 C10	156 N	110.31	130 O	129 C10	157 N	105.89
130 O	129 C10	131 CA	24.66	130 O	129 C10	61 CE1	64.32
130 O	129 C10	156 C	118.60	130 O	129 C10	131 OG	40.06
130 O	129 C10	131 N	12.86	130 O	129 C10	130 CA	15.35
156 NE	129 C10	157 CZ	135.03	156 NE	129 C10	156 CB	38.88
156 NE	129 C10	157 NH1	129.45	156 NE	129 C10	156 NH2	30.21
156 NE	129 C10	157 NE	124.01	156 NE	129 C10	156 CZ	14.78
156 NE	129 C10	156 CG	30.12	156 NE	129 C10	130 C	156.61
156 NE	129 C10	157 CG	96.30	156 NE	129 C10	156 CD	13.58
156 NE	129 C10	301 OH2	124.77	156 NE	129 C10	156 CA	51.78
156 NE	129 C10	130 N	137.57	156 NE	129 C10	157 CD	110.63
156 NE	129 C10	300 OH2	96.57	156 NE	129 C10	156 N	60.83
156 NE	129 C10	157 N	73.81	156 NE	129 C10	131 CA	148.23
156 NE	129 C10	61 CE1	98.63	156 NE	129 C10	156 C	60.95
156 NE	129 C10	131 OG	126.90	156 NE	129 C10	131 N	152.95
156 NE	129 C10	130 CA	150.69	157 CZ	129 C10	156 CB	105.63
157 CZ	129 C10	157 NH1	17.11	157 CZ	129 C10	156 NH2	126.09
157 CZ	129 C10	157 NE	15.28	157 CZ	129 C10	156 CZ	130.33
157 CZ	129 C10	156 CG	122.88	157 CZ	129 C10	130 C	62.29
157 CZ	129 C10	157 CG	41.24	157 CZ	129 C10	156 CD	132.55
157 CZ	129 C10	301 OH2	45.12	157 CZ	129 C10	156 CA	95.71
157 CZ	129 C10	130 N	62.10	157 CZ	129 C10	157 CD	25.52

Fig. 11HHH

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
157 CZ	129 C10	300 OH2	68.31	157 CZ	129 C10	156 N	96.18
157 CZ	129 C10	157 N	71.04	157 CZ	129 C10	131 CA	76.70
157 CZ	129 C10	61 CE1	118.73	157 CZ	129 C10	156 C	81.70
157 CZ	129 C10	131 OG	97.45	157 CZ	129 C10	131 N	70.24
157 CZ	129 C10	130 CA	58.19	156 CB	129 C10	157 NH1	110.45
156 CB	129 C10	156 NH2	63.78	156 CB	129 C10	157 NE	91.08
156 CB	129 C10	156 CZ	49.28	156 CB	129 C10	156 CG	17.98
156 CB	129 C10	130 C	132.31	156 CB	129 C10	157 CG	64.56
156 CB	129 C10	156 CD	28.73	156 CB	129 C10	301 OH2	86.18
156 CB	129 C10	156 CA	12.96	156 CB	129 C10	130 N	106.26
156 CB	129 C10	157 CD	80.49	156 CB	129 C10	300 OH2	59.13
156 CB	129 C10	156 N	25.28	156 CB	129 C10	157 N	36.01
156 CB	129 C10	131 CA	152.31	156 CB	129 C10	61 CE1	100.79
156 CB	129 C10	156 C	24.06	156 CB	129 C10	131 OG	134.81
156 CB	129 C10	131 N	139.97	156 CB	129 C10	130 CA	120.00
157 NH1	129 C10	156 NH2	112.43	157 NH1	129 C10	157 NE	28.96
157 NH1	129 C10	156 CZ	120.33	157 NH1	129 C10	156 CG	128.42
157 NH1	129 C10	130 C	71.94	157 NH1	129 C10	157 CG	47.71
157 NH1	129 C10	156 CD	132.34	157 NH1	129 C10	301 OH2	62.21
157 NH1	129 C10	156 CA	103.30	157 NH1	129 C10	130 N	77.26
157 NH1	129 C10	157 CD	32.51	157 NH1	129 C10	300 OH2	84.03
157 NH1	129 C10	156 N	107.56	157 NH1	129 C10	157 N	79.92
157 NH1	129 C10	131 CA	80.09	157 NH1	129 C10	61 CE1	130.86
157 NH1	129 C10	156 C	88.21	157 NH1	129 C10	131 OG	103.01
157 NH1	129 C10	131 N	77.58	157 NH1	129 C10	130 CA	70.93
156 NH2	129 C10	157 NE	123.87	156 NH2	129 C10	156 CZ	15.71
156 NH2	129 C10	156 CG	59.77	156 NH2	129 C10	130 C	162.13
156 NH2	129 C10	157 CG	101.80	156 NH2	129 C10	156 CD	43.70
156 NH2	129 C10	301 OH2	146.26	156 NH2	129 C10	156 CA	76.29

Fig. 11III

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 NH2	129 C10	130 N	167.66	156 NH2	129 C10	157 CD	110.43
156 NH2	129 C10	300 OH2	122.72	156 NH2	129 C10	156 N	88.44
156 NH2	129 C10	157 N	92.51	156 NH2	129 C10	131 CA	137.44
156 NH2	129 C10	61 CE1	115.18	156 NH2	129 C10	156 C	80.08
156 NH2	129 C10	131 OG	128.43	156 NH2	129 C10	131 N	151.42
156 NH2	129 C10	130 CA	174.26	157 NE	129 C10	156 CZ	123.25
157 NE	129 C10	156 CG	107.92	157 NE	129 C10	130 C	68.73
157 NE	129 C10	157 CG	27.80	157 NE	129 C10	156 CD	118.96
157 NE	129 C10	301 OH2	36.68	157 NE	129 C10	156 CA	80.66
157 NE	129 C10	130 N	61.08	157 NE	129 C10	157 CD	14.03
157 NE	129 C10	300 OH2	55.11	157 NE	129 C10	156 N	80.96
157 NE	129 C10	157 N	55.93	157 NE	129 C10	131 CA	87.33
157 NE	129 C10	61 CE1	118.58	157 NE	129 C10	156 C	67.04
157 NE	129 C10	131 OG	105.37	157 NE	129 C10	131 N	78.28
157 NE	129 C10	130 CA	61.38	156 CZ	129 C10	156 CG	44.06
156 CZ	129 C10	130 C	167.37	156 CZ	129 C10	157 CG	97.23
156 CZ	129 C10	156 CD	28.09	156 CZ	129 C10	301 OH2	134.77
156 CZ	129 C10	156 CA	62.12	156 CZ	129 C10	130 N	152.26
156 CZ	129 C10	157 CD	109.22	156 CZ	129 C10	300 OH2	108.38
156 CZ	129 C10	156 N	73.29	156 CZ	129 C10	157 N	81.09
156 CZ	129 C10	131 CA	147.37	156 CZ	129 C10	61 CE1	108.81
156 CZ	129 C10	156 C	68.18	156 CZ	129 C10	131 OG	131.32
156 CZ	129 C10	131 N	158.46	156 CZ	129 C10	130 CA	165.42
156 CG	129 C10	130 C	132.23	156 CG	129 C10	157 CG	82.21
156 CG	129 C10	156 CD	16.73	156 CG	129 C10	301 OH2	96.10
156 CG	129 C10	156 CA	27.29	156 CG	129 C10	130 N	108.43
156 CG	129 C10	157 CD	98.15	156 CG	129 C10	300 OH2	67.25
156 CG	129 C10	156 N	31.66	156 CG	129 C10	157 N	52.02
156 CG	129 C10	131 CA	143.26	156 CG	129 C10	61 CE1	86.97

Fig. 11JJJ

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CG	129 C10	156 C	41.27	156 CG	129 C10	131 OG	121.33
156 CG	129 C10	131 N	135.84	156 CG	129 C10	130 CA	122.28
130 C	129 C10	157 CG	93.71	130 C	129 C10	156 CD	145.72
130 C	129 C10	301 OH2	51.54	130 C	129 C10	156 CA	120.41
130 C	129 C10	130 N	26.09	130 C	129 C10	157 CD	82.74
130 C	129 C10	300 OH2	74.37	130 C	129 C10	156 N	107.08
130 C	129 C10	157 N	105.36	130 C	129 C10	131 CA	24.69
130 C	129 C10	61 CE1	59.01	130 C	129 C10	156 C	117.73
130 C	129 C10	131 OG	36.68	130 C	129 C10	131 N	10.88
130 C	129 C10	130 CA	12.85	157 CG	129 C10	156 CD	91.48
157 CG	129 C10	301 OH2	48.25	157 CG	129 C10	156 CA	55.79
157 CG	129 C10	130 N	78.79	157 CG	129 C10	157 CD	15.94
157 CG	129 C10	300 OH2	49.12	157 CG	129 C10	156 N	60.57
157 CG	129 C10	157 N	32.31	157 CG	129 C10	131 CA	114.61
157 CG	129 C10	61 CE1	128.79	157 CG	129 C10	156 C	41.00
157 CG	129 C10	131 OG	129.76	157 CG	129 C10	131 N	104.10
157 CG	129 C10	130 CA	83.90	156 CD	129 C10	301 OH2	112.53
156 CD	129 C10	156 CA	40.96	156 CD	129 C10	130 N	124.18
156 CD	129 C10	157 CD	107.03	156 CD	129 C10	300 OH2	83.82
156 CD	129 C10	156 N	48.08	156 CD	129 C10	157 N	64.74
156 CD	129 C10	131 CA	147.34	156 CD	129 C10	61 CE1	91.94
156 CD	129 C10	156 C	52.49	156 CD	129 C10	131 OG	124.07
156 CD	129 C10	131 N	145.89	156 CD	129 C10	130 CA	137.64
301 OH2	129 C10	156 CA	73.22	301 OH2	129 C10	130 N	30.88
301 OH2	129 C10	157 CD	45.62	301 OH2	129 C10	300 OH2	28.95
301 OH2	129 C10	156 N	64.48	301 OH2	129 C10	157 N	54.04
301 OH2	129 C10	131 CA	76.14	301 OH2	129 C10	61 CE1	83.86
301 OH2	129 C10	156 C	66.78	301 OH2	129 C10	131 OG	83.36
301 OH2	129 C10	131 N	62.32	301 OH2	129 C10	130 CA	39.23

Fig. 11KKK

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
156 CA	129 C10	130 N	94.35	156 CA	129 C10	157 CD	71.57
156 CA	129 C10	300 OH2	46.46	156 CA	129 C10	156 N	15.33
156 CA	129 C10	157 N	24.73	156 CA	129 C10	131 CA	142.75
156 CA	129 C10	61 CE1	98.98	156 CA	129 C10	156 C	15.22
156 CA	129 C10	131 OG	130.58	156 CA	129 C10	131 N	129.08
156 CA	129 C10	130 CA	107.81	130 N	129 C10	157 CD	73.28
130 N	129 C10	300 OH2	48.70	130 N	129 C10	156 N	81.10
130 N	129 C10	157 N	81.45	130 N	129 C10	131 CA	49.60
130 N	129 C10	61 CE1	57.71	130 N	129 C10	156 C	92.99
130 N	129 C10	131 OG	52.61	130 N	129 C10	131 N	35.27
130 N	129 C10	130 CA	14.01	157 CD	129 C10	300 OH2	56.55
157 CD	129 C10	156 N	75.09	157 CD	129 C10	157 N	47.54
157 CD	129 C10	131 CA	100.99	157 CD	129 C10	61 CE1	129.46
157 CD	129 C10	156 C	56.91	157 CD	129 C10	131 OG	119.39
157 CD	129 C10	131 N	92.30	157 CD	129 C10	130 CA	74.96
300 OH2	129 C10	156 N	35.77	300 OH2	129 C10	157 N	34.36
300 OH2	129 C10	131 CA	98.29	300 OH2	129 C10	61 CE1	80.57
300 OH2	129 C10	156 C	44.60	300 OH2	129 C10	131 OG	96.41
300 OH2	129 C10	131 N	83.97	300 OH2	129 C10	130 CA	61.58
156 N	129 C10	157 N	28.54	156 N	129 C10	131 CA	127.93
156 N	129 C10	61 CE1	85.38	156 N	129 C10	156 C	25.75
156 N	129 C10	131 OG	115.55	156 N	129 C10	131 N	114.82
156 N	129 C10	130 CA	94.97	157 N	129 C10	131 CA	130.05
157 N	129 C10	61 CE1	109.04	157 N	129 C10	156 C	12.98
157 N	129 C10	131 OG	130.70	157 N	129 C10	131 N	115.92
157 N	129 C10	130 CA	92.69	131 CA	129 C10	61 CE1	56.75
131 CA	129 C10	156 C	142.34	131 CA	129 C10	131 OG	23.31
131 CA	129 C10	131 N	14.35	131 CA	129 C10	130 CA	37.42
61 CE1	129 C10	156 C	111.01	61 CE1	129 C10	131 OG	34.45

Fig. 11LLL

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CE1	129 C10	131 N	54.64	61 CE1	129 C10	130 CA	60.66
156 C	129 C10	131 OG	138.61	156 C	129 C10	131 N	128.02
156 C	129 C10	130 CA	104.93	131 OG	129 C10	131 N	27.34
131 OG	129 C10	130 CA	45.86	131 N	129 C10	130 CA	23.23

Fig. 12A

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 C	129 N	129 CA	120.79	128 C	129 N	128 O	27.54
128 C	129 N	129 C	144.53	128 C	129 N	129 CB	120.04
128 C	129 N	128 CA	34.33	128 C	129 N	129 O	163.28
128 C	129 N	128 CB	51.26	128 C	129 N	130 N	127.69
128 C	129 N	128 N	20.30	128 C	129 N	128 CG2	46.96
128 C	129 N	129 OG	120.46	128 C	129 N	321 OH2	67.29
128 C	129 N	152 SG	72.21	128 C	129 N	128 CG1	52.53
128 C	129 N	130 CA	133.61	128 C	129 N	152 N	74.93
129 CA	129 N	128 O	93.25	129 CA	129 N	129 C	38.96
129 CA	129 N	129 CB	37.48	129 CA	129 N	128 CA	155.12
129 CA	129 N	129 O	60.71	129 CA	129 N	128 CB	148.96
129 CA	129 N	130 N	39.47	129 CA	129 N	128 N	138.58
129 CA	129 N	128 CG2	125.62	129 CA	129 N	129 OG	25.11
129 CA	129 N	321 OH2	54.02	129 CA	129 N	152 SG	98.20
129 CA	129 N	128 CG1	158.20	129 CA	129 N	130 CA	48.82
129 CA	129 N	152 N	127.86	128 O	129 N	129 C	122.01
128 O	129 N	129 CB	98.73	128 O	129 N	128 CA	61.87
128 O	129 N	129 O	148.34	128 O	129 N	128 CB	74.70
128 O	129 N	130 N	107.34	128 O	129 N	128 N	46.59
128 O	129 N	128 CG2	61.54	128 O	129 N	129 OG	95.73
128 O	129 N	321 OH2	40.06	128 O	129 N	152 SG	73.56
128 O	129 N	128 CG1	78.13	128 O	129 N	130 CA	116.77
128 O	129 N	152 N	91.39	129 C	129 N	129 CB	64.49
129 C	129 N	128 CA	155.27	129 C	129 N	129 O	26.53
129 C	129 N	128 CB	125.78	129 C	129 N	130 N	17.05
129 C	129 N	128 N	162.70	129 C	129 N	128 CG2	113.45
129 C	129 N	129 OG	55.95	129 C	129 N	321 OH2	88.92
129 C	129 N	152 SG	128.56	129 C	129 N	128 CG1	131.44
129 C	129 N	130 CA	15.50	129 C	129 N	152 N	139.63
129 CB	129 N	128 CA	140.15	129 CB	129 N	129 O	72.14
129 CB	129 N	128 CB	169.60	129 CB	129 N	130 N	73.09
129 CB	129 N	128 N	125.29	129 CB	129 N	128 CG2	156.56
129 CB	129 N	129 OG	12.50	129 CB	129 N	321 OH2	63.01
129 CB	129 N	152 SG	64.73	129 CB	129 N	128 CG1	162.91
129 CB	129 N	130 CA	79.04	129 CB	129 N	152 N	90.53
128 CA	129 N	129 O	142.14	128 CA	129 N	128 CB	29.52
128 CA	129 N	130 N	143.57	128 CA	129 N	128 N	17.97
128 CA	129 N	128 CG2	44.08	128 CA	129 N	129 OG	147.55
128 CA	129 N	321 OH2	101.36	128 CA	129 N	152 SG	76.07
128 CA	129 N	128 CG1	24.72	128 CA	129 N	130 CA	140.21
128 CA	129 N	152 N	58.11	129 O	129 N	128 CB	117.66
129 O	129 N	130 N	41.16	129 O	129 N	128 N	160.10
129 O	129 N	128 CG2	117.27	129 O	129 N	129 OG	68.68

Fig. 12B

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 O	129 N	321 OH2	114.01	129 O	129 N	152 SG	124.51
129 O	129 N	128 CG1	118.99	129 O	129 N	130 CA	32.68
129 O	129 N	152 N	118.35	128 CB	129 N	130 N	116.32
128 CB	129 N	128 N	44.43	128 CB	129 N	128 CG2	23.99
128 CB	129 N	129 OG	169.67	128 CB	129 N	321 OH2	112.84
128 CB	129 N	152 SG	105.29	128 CB	129 N	128 CG1	9.24
128 CB	129 N	130 CA	111.03	128 CB	129 N	152 N	81.70
130 N	129 N	128 N	145.82	130 N	129 N	128 CG2	99.56
130 N	129 N	129 OG	62.24	130 N	129 N	321 OH2	79.71
130 N	129 N	152 SG	137.22	130 N	129 N	128 CG1	123.96
130 N	129 N	130 CA	11.53	130 N	129 N	152 N	156.54
128 N	129 N	128 CG2	51.30	128 N	129 N	129 OG	130.50
128 N	129 N	321 OH2	84.63	128 N	129 N	152 SG	65.04
128 N	129 N	128 CG1	41.72	128 N	129 N	130 CA	148.38
128 N	129 N	152 N	57.61	128 CG2	129 N	129 OG	146.71
128 CG2	129 N	321 OH2	94.01	128 CG2	129 N	152 SG	116.23
128 CG2	129 N	128 CG1	32.95	128 CG2	129 N	130 CA	98.00
128 CG2	129 N	152 N	101.82	129 OG	129 N	321 OH2	57.00
129 OG	129 N	152 SG	75.03	129 OG	129 N	128 CG1	172.22
129 OG	129 N	130 CA	69.44	129 OG	129 N	152 N	102.77
321 OH2	129 N	152 SG	75.36	321 OH2	129 N	128 CG1	117.66
321 OH2	129 N	130 CA	91.20	321 OH2	129 N	152 N	108.16
152 SG	129 N	128 CG1	98.46	152 SG	129 N	130 CA	143.66
152 SG	129 N	152 N	34.95	128 CG1	129 N	130 CA	117.52
128 CG1	129 N	152 N	72.87	130 CA	129 N	152 N	151.01
129 N	129 CA	129 CB	107.57	129 N	129 CA	129 C	104.87
129 N	129 CA	129 O	87.62	129 N	129 CA	128 C	28.26
129 N	129 CA	129 OG	140.32	129 N	129 CA	130 N	118.72
129 N	129 CA	128 O	55.09	129 N	129 CA	321 OH2	104.92
129 N	129 CA	128 CA	15.61	129 N	129 CA	130 CA	114.75
129 N	129 CA	128 CB	21.28	129 N	129 CA	130 C	129.70
129 N	129 CA	128 CG2	39.58	129 N	129 CA	128 N	29.78
129 N	129 CA	152 SG	64.48	129 N	129 CA	130 O	143.45
129 N	129 CA	61 NE2	113.16	129 N	129 CA	130 CB	111.76
129 N	129 CA	61 CE1	116.08	129 N	129 CA	131 N	123.98
129 CB	129 CA	129 C	111.81	129 CB	129 CA	129 O	99.15
129 CB	129 CA	128 C	110.33	129 CB	129 CA	129 OG	32.88
129 CB	129 CA	130 N	123.38	129 CB	129 CA	128 O	108.07
129 CB	129 CA	321 OH2	86.88	129 CB	129 CA	128 CA	109.80
129 CB	129 CA	130 CA	120.13	129 CB	129 CA	128 CB	128.03
129 CB	129 CA	130 C	102.69	129 CB	129 CA	128 CG2	142.36
129 CB	129 CA	128 N	103.98	129 CB	129 CA	152 SG	50.11
129 CB	129 CA	130 O	97.48	129 CB	129 CA	61 NE2	26.48
129 CB	129 CA	130 CB	132.53	129 CB	129 CA	61 CE1	41.74

Fig. 12C

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 CB	129 CA	131 N	95.92	129 C	129 CA	129 O	26.49
129 C	129 CA	128 C	125.36	129 C	129 CA	129 OG	97.82
129 C	129 CA	130 N	28.62	129 C	129 CA	128 O	139.49
129 C	129 CA	321 OH2	137.54	129 C	129 CA	128 CA	116.52
129 C	129 CA	130 CA	19.07	129 C	129 CA	128 CB	98.68
129 C	129 CA	130 C	25.23	129 C	129 CA	128 CG2	97.56
129 C	129 CA	128 N	130.67	129 C	129 CA	152 SG	145.98
129 C	129 CA	130 O	39.70	129 C	129 CA	61 NE2	85.55
129 C	129 CA	130 CB	32.65	129 C	129 CA	61 CE1	70.21
129 C	129 CA	131 N	20.79	129 O	129 CA	128 C	114.21
129 O	129 CA	129 OG	99.73	129 O	129 CA	130 N	55.04
129 O	129 CA	128 O	138.69	129 O	129 CA	321 OH2	163.86
129 O	129 CA	128 CA	102.32	129 O	129 CA	130 CA	45.51
129 O	129 CA	128 CB	89.86	129 O	129 CA	130 C	48.08
129 O	129 CA	128 CG2	97.10	129 O	129 CA	128 N	117.21
129 O	129 CA	152 SG	120.07	129 O	129 CA	130 O	61.95
129 O	129 CA	61 NE2	73.75	129 O	129 CA	130 CB	58.00
129 O	129 CA	61 CE1	59.90	129 O	129 CA	131 N	37.87
128 C	129 CA	129 OG	135.56	128 C	129 CA	130 N	126.00
128 C	129 CA	128 O	26.83	128 C	129 CA	321 OH2	76.99
128 C	129 CA	128 CA	12.65	128 C	129 CA	130 CA	127.11
128 C	129 CA	128 CB	26.70	128 C	129 CA	130 C	145.28
128 C	129 CA	128 CG2	32.34	128 C	129 CA	128 N	6.42
128 C	129 CA	152 SG	60.24	128 C	129 CA	130 O	152.05
128 C	129 CA	61 NE2	127.94	128 C	129 CA	130 CB	116.95
128 C	129 CA	61 CE1	137.23	128 C	129 CA	131 N	146.15
129 OG	129 CA	130 N	96.55	129 OG	129 CA	128 O	120.02
129 OG	129 CA	321 OH2	77.24	129 OG	129 CA	128 CA	139.71
129 OG	129 CA	130 CA	97.04	129 OG	129 CA	128 CB	159.61
129 OG	129 CA	130 C	79.01	129 OG	129 CA	128 CG2	163.15
129 OG	129 CA	128 N	129.39	129 OG	129 CA	152 SG	78.47
129 OG	129 CA	130 O	69.43	129 OG	129 CA	61 NE2	36.42
129 OG	129 CA	130 CB	104.96	129 OG	129 CA	61 CE1	43.65
129 OG	129 CA	131 N	77.43	130 N	129 CA	128 O	124.27
130 N	129 CA	321 OH2	109.20	130 N	129 CA	128 CA	123.71
130 N	129 CA	130 CA	9.56	130 N	129 CA	128 CB	103.67
130 N	129 CA	130 C	21.19	130 N	129 CA	128 CG2	93.66
130 N	129 CA	128 N	132.41	130 N	129 CA	152 SG	172.64
130 N	129 CA	130 O	27.13	130 N	129 CA	61 NE2	101.36
130 N	129 CA	130 CB	9.16	130 N	129 CA	61 CE1	87.30
130 N	129 CA	131 N	31.16	128 O	129 CA	321 OH2	50.51
128 O	129 CA	128 CA	39.48	128 O	129 CA	130 CA	130.46
128 O	129 CA	128 CB	48.88	128 O	129 CA	130 C	144.77
128 O	129 CA	128 CG2	43.40	128 O	129 CA	128 N	26.59

Fig. 12D

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 O	129 CA	152 SG	63.10	128 O	129 CA	130 O	139.99
128 O	129 CA	61 NE2	133.39	128 O	129 CA	130 CB	115.79
128 O	129 CA	61 CE1	148.23	128 O	129 CA	131 N	155.14
321 OH2	129 CA	128 CA	89.51	321 OH2	129 CA	130 CA	118.66
321 OH2	129 CA	128 CB	98.23	321 OH2	129 CA	130 C	116.07
321 OH2	129 CA	128 CG2	86.77	321 OH2	129 CA	128 N	75.21
321 OH2	129 CA	152 SG	75.21	321 OH2	129 CA	130 O	102.56
321 OH2	129 CA	61 NE2	109.32	321 OH2	129 CA	130 CB	107.08
321 OH2	129 CA	61 CE1	120.52	321 OH2	129 CA	131 N	126.96
128 CA	129 CA	130 CA	122.36	128 CA	129 CA	128 CB	20.07
128 CA	129 CA	130 C	139.61	128 CA	129 CA	128 CG2	33.12
128 CA	129 CA	128 N	14.98	128 CA	129 CA	152 SG	61.32
128 CA	129 CA	130 O	150.79	128 CA	129 CA	61 NE2	122.18
128 CA	129 CA	130 CB	115.31	128 CA	129 CA	61 CE1	128.42
128 CA	129 CA	131 N	136.87	130 CA	129 CA	128 CB	102.46
130 CA	129 CA	130 C	18.18	130 CA	129 CA	128 CG2	95.25
130 CA	129 CA	128 N	133.43	130 CA	129 CA	152 SG	164.43
130 CA	129 CA	130 O	29.00	130 CA	129 CA	61 NE2	96.05
130 CA	129 CA	130 CB	15.28	130 CA	129 CA	61 CE1	81.29
130 CA	129 CA	131 N	24.72	128 CB	129 CA	130 C	120.10
128 CB	129 CA	128 CG2	18.76	128 CB	129 CA	128 N	32.16
128 CB	129 CA	152 SG	81.15	128 CB	129 CA	130 O	130.72
128 CB	129 CA	61 NE2	133.74	128 CB	129 CA	130 CB	95.39
128 CB	129 CA	61 CE1	133.86	128 CB	129 CA	131 N	119.46
130 C	129 CA	128 CG2	113.38	130 C	129 CA	128 N	151.57
130 C	129 CA	152 SG	151.58	130 C	129 CA	130 O	14.51
130 C	129 CA	61 NE2	80.19	130 C	129 CA	130 CB	30.24
130 C	129 CA	61 CE1	66.35	130 C	129 CA	131 N	12.63
128 CG2	129 CA	128 N	38.75	128 CG2	129 CA	152 SG	92.47
128 CG2	129 CA	130 O	120.11	128 CG2	129 CA	61 NE2	152.50
128 CG2	129 CA	130 CB	84.63	128 CG2	129 CA	61 CE1	150.72
128 CG2	129 CA	131 N	117.22	128 N	129 CA	152 SG	53.87
128 N	129 CA	130 O	158.21	128 N	129 CA	61 NE2	122.39
128 N	129 CA	130 CB	123.35	128 N	129 CA	61 CE1	132.74
128 N	129 CA	131 N	151.36	152 SG	129 CA	130 O	147.35
152 SG	129 CA	61 NE2	71.40	152 SG	129 CA	130 CB	176.16
152 SG	129 CA	61 CE1	85.36	152 SG	129 CA	131 N	141.50
130 O	129 CA	61 NE2	79.09	130 O	129 CA	130 CB	35.78
130 O	129 CA	61 CE1	67.48	130 O	129 CA	131 N	24.46
61 NE2	129 CA	130 CB	110.27	61 NE2	129 CA	61 CE1	15.34
61 NE2	129 CA	131 N	71.34	130 CB	129 CA	61 CE1	95.93
130 CB	129 CA	131 N	39.40	61 CE1	129 CA	131 N	56.62
129 OG	129 CB	129 CA	111.19	129 OG	129 CB	129 N	146.00
129 OG	129 CB	129 C	96.69	129 OG	129 CB	129 O	105.98

Fig. 12E

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 OG	129 CB	128 C	142.68	129 OG	129 CB	321 OH2	82.02
129 OG	129 CB	128 O	124.31	129 OG	129 CB	130 N	83.03
129 OG	129 CB	61 NE2	65.74	129 OG	129 CB	152 SG	124.02
129 OG	129 CB	61 CE1	65.92	129 OG	129 CB	128 CA	155.37
129 OG	129 CB	61 CD2	73.86	129 OG	129 CB	130 CA	81.35
129 OG	129 CB	130 C	66.70	129 OG	129 CB	152 CB	123.31
129 OG	129 CB	130 O	54.67	129 OG	129 CB	61 ND1	72.12
129 OG	129 CB	128 N	147.39	129 OG	129 CB	156 N	67.44
129 OG	129 CB	128 CB	149.20	129 CA	129 CB	129 N	34.95
129 CA	129 CB	129 C	34.15	129 CA	129 CB	129 O	51.04
129 CA	129 CB	128 C	43.64	129 CA	129 CB	321 OH2	67.33
129 CA	129 CB	128 O	47.59	129 CA	129 CB	130 N	35.50
129 CA	129 CB	61 NE2	142.46	129 CA	129 CB	152 SG	112.75
129 CA	129 CB	61 CE1	123.54	129 CA	129 CB	128 CA	51.62
129 CA	129 CB	61 CD2	147.70	129 CA	129 CB	130 CA	43.82
129 CA	129 CB	130 C	60.38	129 CA	129 CB	152 CB	122.06
129 CA	129 CB	130 O	65.67	129 CA	129 CB	61 ND1	124.07
129 CA	129 CB	128 N	59.77	129 CA	129 CB	156 N	97.93
129 CA	129 CB	128 CB	39.21	129 N	129 CB	129 C	57.02
129 N	129 CB	129 O	59.18	129 N	129 CB	128 C	20.56
129 N	129 CB	321 OH2	79.51	129 N	129 CB	128 O	39.09
129 N	129 CB	130 N	66.61	129 N	129 CB	61 NE2	138.67
129 N	129 CB	152 SG	82.30	129 N	129 CB	61 CE1	127.89
129 N	129 CB	128 CA	19.97	129 N	129 CB	61 CD2	134.29
129 N	129 CB	130 CA	71.51	129 N	129 CB	130 C	88.42
129 N	129 CB	152 CB	88.20	129 N	129 CB	130 O	97.34
129 N	129 CB	61 ND1	123.89	129 N	129 CB	128 N	33.07
129 N	129 CB	156 N	106.20	129 N	129 CB	128 CB	5.85
129 C	129 CB	129 O	23.30	129 C	129 CB	128 C	73.51
129 C	129 CB	321 OH2	94.70	129 C	129 CB	128 O	81.55
129 C	129 CB	130 N	16.89	129 C	129 CB	61 NE2	108.50
129 C	129 CB	152 SG	138.53	129 C	129 CB	61 CE1	89.48
129 C	129 CB	128 CA	76.97	129 C	129 CB	61 CD2	115.12
129 C	129 CB	130 CA	15.35	129 C	129 CB	130 C	31.52
129 C	129 CB	152 CB	138.56	129 C	129 CB	130 O	42.13
129 C	129 CB	61 ND1	90.57	129 C	129 CB	128 N	89.00
129 C	129 CB	156 N	122.00	129 C	129 CB	128 CB	62.81
129 O	129 CB	128 C	79.32	129 O	129 CB	321 OH2	116.77
129 O	129 CB	128 O	93.75	129 O	129 CB	130 N	38.94
129 O	129 CB	61 NE2	92.53	129 O	129 CB	152 SG	128.38
129 O	129 CB	61 CE1	74.69	129 O	129 CB	128 CA	77.58
129 O	129 CB	61 CD2	96.66	129 O	129 CB	130 CA	32.31
129 O	129 CB	130 C	40.96	129 O	129 CB	152 CB	121.40
129 O	129 CB	130 O	54.24	129 O	129 CB	61 ND1	73.82

Fig. 12F

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 O	129 CB	128 N	91.78	129 O	129 CB	156 N	145.25
129 O	129 CB	128 CB	64.74	128 C	129 CB	321 OH2	63.58
128 C	129 CB	128 O	20.52	128 C	129 CB	130 N	79.02
128 C	129 CB	61 NE2	151.57	128 C	129 CB	152 SG	69.13
128 C	129 CB	61 CE1	146.86	128 C	129 CB	128 CA	12.72
128 C	129 CB	61 CD2	143.18	128 C	129 CB	130 CA	86.34
128 C	129 CB	130 C	103.38	128 C	129 CB	152 CB	79.39
128 C	129 CB	130 O	109.26	128 C	129 CB	61 ND1	141.82
128 C	129 CB	128 N	16.15	128 C	129 CB	156 N	87.06
128 C	129 CB	128 CB	15.85	321 OH2	129 CB	128 O	43.24
321 OH2	129 CB	130 N	83.01	321 OH2	129 CB	61 NE2	141.72
321 OH2	129 CB	152 SG	84.51	321 OH2	129 CB	61 CE1	147.94
321 OH2	129 CB	128 CA	74.92	321 OH2	129 CB	61 CD2	143.18
321 OH2	129 CB	130 CA	93.24	321 OH2	129 CB	130 C	99.30
321 OH2	129 CB	152 CB	100.66	321 OH2	129 CB	130 O	91.14
321 OH2	129 CB	61 ND1	154.04	321 OH2	129 CB	128 N	65.48
321 OH2	129 CB	156 N	30.68	321 OH2	129 CB	128 CB	77.45
128 O	129 CB	130 N	81.21	128 O	129 CB	61 NE2	165.75
128 O	129 CB	152 SG	69.68	128 O	129 CB	61 CE1	166.98
128 O	129 CB	128 CA	31.77	128 O	129 CB	61 CD2	155.34
128 O	129 CB	130 CA	90.78	128 O	129 CB	130 C	106.20
128 O	129 CB	152 CB	83.87	128 O	129 CB	130 O	107.32
128 O	129 CB	61 ND1	162.34	128 O	129 CB	128 N	25.03
128 O	129 CB	156 N	67.18	128 O	129 CB	128 CB	35.57
130 N	129 CB	61 NE2	111.40	130 N	129 CB	152 SG	148.09
130 N	129 CB	61 CE1	92.94	130 N	129 CB	128 CA	85.64
130 N	129 CB	61 CD2	120.18	130 N	129 CB	130 CA	10.69
130 N	129 CB	130 C	25.14	130 N	129 CB	152 CB	153.62
130 N	129 CB	130 O	30.86	130 N	129 CB	61 ND1	95.78
130 N	129 CB	128 N	95.17	130 N	129 CB	156 N	107.25
130 N	129 CB	128 CB	71.96	61 NE2	129 CB	152 SG	96.45
61 NE2	129 CB	61 CE1	19.04	61 NE2	129 CB	128 CA	138.89
61 NE2	129 CB	61 CD2	10.42	61 NE2	129 CB	130 CA	101.30
61 NE2	129 CB	130 C	86.85	61 NE2	129 CB	152 CB	81.94
61 NE2	129 CB	130 O	86.71	61 NE2	129 CB	61 ND1	18.71
61 NE2	129 CB	128 N	141.98	61 NE2	129 CB	156 N	113.07
61 NE2	129 CB	128 CB	140.16	152 SG	129 CB	61 CE1	112.63
152 SG	129 CB	128 CA	62.74	152 SG	129 CB	61 CD2	86.40
152 SG	129 CB	130 CA	153.66	152 SG	129 CB	130 C	169.18
152 SG	129 CB	152 CB	16.42	152 SG	129 CB	130 O	175.63
152 SG	129 CB	61 ND1	107.92	152 SG	129 CB	128 N	52.98
152 SG	129 CB	156 N	73.73	152 SG	129 CB	128 CB	76.71
61 CE1	129 CB	128 CA	136.69	61 CE1	129 CB	61 CD2	27.27
61 CE1	129 CB	130 CA	82.61	61 CE1	129 CB	130 C	69.07

Fig. 12G

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
61 CE1	129 CB	152 CB	96.91	61 CE1	129 CB	130 O	71.04
61 CE1	129 CB	61 ND1	6.48	61 CE1	129 CB	128 N	146.49
61 CE1	129 CB	156 N	125.82	61 CE1	129 CB	128 CB	131.48
128 CA	129 CB	61 CD2	130.52	128 CA	129 CB	130 CA	91.29
128 CA	129 CB	130 C	108.29	128 CA	129 CB	152 CB	70.44
128 CA	129 CB	130 O	116.51	128 CA	129 CB	61 ND1	130.96
128 CA	129 CB	128 N	14.42	128 CA	129 CB	156 N	95.45
128 CA	129 CB	128 CB	14.16	61 CD2	129 CB	130 CA	109.75
61 CD2	129 CB	130 C	96.23	61 CD2	129 CB	152 CB	71.62
61 CD2	129 CB	130 O	96.89	61 CD2	129 CB	61 ND1	24.75
61 CD2	129 CB	128 N	131.97	61 CD2	129 CB	156 N	112.75
61 CD2	129 CB	128 CB	134.43	130 CA	129 CB	130 C	17.11
130 CA	129 CB	152 CB	152.93	130 CA	129 CB	130 O	26.79
130 CA	129 CB	61 ND1	85.22	130 CA	129 CB	128 N	102.32
130 CA	129 CB	156 N	115.76	130 CA	129 CB	128 CB	77.19
130 C	129 CB	152 CB	158.79	130 C	129 CB	130 O	13.35
130 C	129 CB	61 ND1	72.80	130 C	129 CB	128 N	119.41
130 C	129 CB	156 N	114.47	130 C	129 CB	128 CB	94.15
152 CB	129 CB	130 O	167.73	152 CB	129 CB	61 ND1	91.89
152 CB	129 CB	128 N	63.82	152 CB	129 CB	156 N	86.55
152 CB	129 CB	128 CB	83.27	130 O	129 CB	61 ND1	75.93
130 O	129 CB	128 N	125.32	130 O	129 CB	156 N	102.27
130 O	129 CB	128 CB	102.78	61 ND1	129 CB	128 N	140.14
61 ND1	129 CB	156 N	129.82	61 ND1	129 CB	128 CB	126.97
128 N	129 CB	156 N	82.30	128 N	129 CB	128 CB	27.29
156 N	129 CB	128 CB	102.67	129 CB	129 OG	129 CA	35.93
129 CB	129 OG	129 C	55.83	129 CB	129 OG	61 NE2	90.82
129 CB	129 OG	321 OH2	75.06	129 CB	129 OG	130 N	74.36
129 CB	129 OG	129 N	21.50	129 CB	129 OG	61 CE1	93.44
129 CB	129 OG	129 O	52.38	129 CB	129 OG	128 C	26.27
129 CB	129 OG	128 O	40.57	129 CB	129 OG	61 CD2	88.78
129 CB	129 OG	130 O	110.68	129 CB	129 OG	130 C	97.40
129 CB	129 OG	130 CA	81.64	129 CB	129 OG	152 SG	42.18
129 CB	129 OG	156 N	97.41	129 CB	129 OG	61 ND1	92.27
129 CB	129 OG	131 OG	108.36	129 CB	129 OG	131 N	96.58
129 CB	129 OG	61 CG	89.83	129 CB	129 OG	156 CB	124.06
129 CA	129 OG	129 C	29.94	129 CA	129 OG	61 NE2	117.15
129 CA	129 OG	321 OH2	61.56	129 CA	129 OG	130 N	42.09
129 CA	129 OG	129 N	14.57	129 CA	129 OG	61 CE1	109.11
129 CA	129 OG	129 O	39.75	129 CA	129 OG	128 C	22.10
129 CA	129 OG	128 O	31.97	129 CA	129 OG	61 CD2	118.07
129 CA	129 OG	130 O	80.66	129 CA	129 OG	130 C	70.81
129 CA	129 OG	130 CA	52.67	129 CA	129 OG	152 SG	72.56
129 CA	129 OG	156 N	95.97	129 CA	129 OG	61 ND1	109.21

Fig. 12H

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 CA	129 OG	131 OG	102.95	129 CA	129 OG	131 N	76.22
129 CA	129 OG	61 CG	114.16	129 CA	129 OG	156 CB	117.71
129 C	129 OG	61 NE2	104.72	129 C	129 OG	321 OH2	84.76
129 C	129 OG	130 N	20.59	129 C	129 OG	129 N	39.91
129 C	129 OG	61 CE1	88.98	129 C	129 OG	129 O	17.97
129 C	129 OG	128 C	51.69	129 C	129 OG	128 O	61.32
129 C	129 OG	61 CD2	109.15	129 C	129 OG	130 O	54.94
129 C	129 OG	130 C	42.62	129 C	129 OG	130 CA	25.81
129 C	129 OG	152 SG	97.67	129 C	129 OG	156 N	120.43
129 C	129 OG	61 ND1	89.98	129 C	129 OG	131 OG	74.01
129 C	129 OG	131 N	46.38	129 C	129 OG	61 CG	100.28
129 C	129 OG	156 CB	133.74	61 NE2	129 OG	321 OH2	154.78
61 NE2	129 OG	130 N	116.43	61 NE2	129 OG	129 N	107.95
61 NE2	129 OG	61 CE1	21.03	61 NE2	129 OG	129 O	86.93
61 NE2	129 OG	128 C	117.08	61 NE2	129 OG	128 O	130.38
61 NE2	129 OG	61 CD2	7.25	61 NE2	129 OG	130 O	102.81
61 NE2	129 OG	130 C	97.21	61 NE2	129 OG	130 CA	106.55
61 NE2	129 OG	152 SG	84.61	61 NE2	129 OG	156 N	130.20
61 NE2	129 OG	61 ND1	18.93	61 NE2	129 OG	131 OG	54.38
61 NE2	129 OG	131 N	83.84	61 NE2	129 OG	61 CG	4.84
61 NE2	129 OG	156 CB	121.14	321 OH2	129 OG	130 N	80.29
321 OH2	129 OG	129 N	64.54	321 OH2	129 OG	61 CE1	168.50
321 OH2	129 OG	129 O	100.02	321 OH2	129 OG	128 C	51.19
321 OH2	129 OG	128 O	35.36	321 OH2	129 OG	61 CD2	147.83
321 OH2	129 OG	130 O	101.72	321 OH2	129 OG	130 C	105.14
321 OH2	129 OG	130 CA	92.19	321 OH2	129 OG	152 SG	70.85
321 OH2	129 OG	156 N	35.71	321 OH2	129 OG	61 ND1	167.13
321 OH2	129 OG	131 OG	149.82	321 OH2	129 OG	131 N	117.98
321 OH2	129 OG	61 CG	157.83	321 OH2	129 OG	156 CB	56.48
130 N	129 OG	129 N	55.44	130 N	129 OG	61 CE1	97.07
130 N	129 OG	129 O	35.62	130 N	129 OG	128 C	63.58
130 N	129 OG	128 O	68.05	130 N	129 OG	61 CD2	122.40
130 N	129 OG	130 O	38.58	130 N	129 OG	130 C	30.31
130 N	129 OG	130 CA	12.71	130 N	129 OG	152 SG	114.46
130 N	129 OG	156 N	113.09	130 N	129 OG	61 ND1	98.69
130 N	129 OG	131 OG	72.27	130 N	129 OG	131 N	39.83
130 N	129 OG	61 CG	111.60	130 N	129 OG	156 CB	117.88
129 N	129 OG	61 CE1	104.69	129 N	129 OG	129 O	43.83
129 N	129 OG	128 C	14.79	129 N	129 OG	128 O	29.99
129 N	129 OG	61 CD2	107.41	129 N	129 OG	130 O	93.68
129 N	129 OG	130 C	82.43	129 N	129 OG	130 CA	64.85
129 N	129 OG	152 SG	59.05	129 N	129 OG	156 N	95.31
129 N	129 OG	61 ND1	104.21	129 N	129 OG	131 OG	107.44
129 N	129 OG	131 N	85.58	129 N	129 OG	61 CG	105.86

Fig. 12I

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 N	129 OG	156 CB	120.37	61 CE1	129 OG	129 O	72.40
61 CE1	129 OG	128 C	117.60	61 CE1	129 OG	128 O	133.34
61 CE1	129 OG	61 CD2	28.22	61 CE1	129 OG	130 O	82.37
61 CE1	129 OG	130 C	76.18	61 CE1	129 OG	130 CA	86.28
61 CE1	129 OG	152 SG	100.55	61 CE1	129 OG	156 N	149.69
61 CE1	129 OG	61 ND1	2.32	61 CE1	129 OG	131 OG	34.33
61 CE1	129 OG	131 N	62.81	61 CE1	129 OG	61 CG	16.53
61 CE1	129 OG	156 CB	133.17	129 O	129 OG	128 C	58.18
129 O	129 OG	128 O	71.30	129 O	129 OG	61 CD2	91.19
129 O	129 OG	130 O	60.86	129 O	129 OG	130 C	46.38
129 O	129 OG	130 CA	34.94	129 O	129 OG	152 SG	93.71
129 O	129 OG	156 N	135.41	129 O	129 OG	61 ND1	73.15
129 O	129 OG	131 OG	64.02	129 O	129 OG	131 N	44.23
129 O	129 OG	61 CG	82.58	129 O	129 OG	156 CB	151.70
128 C	129 OG	128 O	15.88	128 C	129 OG	61 CD2	114.91
128 C	129 OG	130 O	102.00	128 C	129 OG	130 C	92.86
128 C	129 OG	130 CA	74.67	128 C	129 OG	152 SG	52.26
128 C	129 OG	156 N	80.57	128 C	129 OG	61 ND1	116.80
128 C	129 OG	131 OG	122.09	128 C	129 OG	131 N	98.07
128 C	129 OG	61 CG	115.95	128 C	129 OG	156 CB	106.01
128 O	129 OG	61 CD2	126.88	128 O	129 OG	130 O	104.05
128 O	129 OG	130 C	98.37	128 O	129 OG	130 CA	80.42
128 O	129 OG	152 SG	54.32	128 O	129 OG	156 N	65.62
128 O	129 OG	61 ND1	132.44	128 O	129 OG	131 OG	134.92
128 O	129 OG	131 N	106.49	128 O	129 OG	61 CG	130.05
128 O	129 OG	156 CB	90.40	61 CD2	129 OG	130 O	110.03
61 CD2	129 OG	130 C	104.38	61 CD2	129 OG	130 CA	113.11
61 CD2	129 OG	152 SG	78.47	61 CD2	129 OG	156 N	123.65
61 CD2	129 OG	61 ND1	26.07	61 CD2	129 OG	131 OG	61.60
61 CD2	129 OG	131 N	90.99	61 CD2	129 OG	61 CG	11.75
61 CD2	129 OG	156 CB	117.10	130 O	129 OG	130 C	14.76
130 O	129 OG	130 CA	29.15	130 O	129 OG	152 SG	152.55
130 O	129 OG	156 N	119.30	130 O	129 OG	61 ND1	84.66
130 O	129 OG	131 OG	48.43	130 O	129 OG	131 N	24.07
130 O	129 OG	61 CG	98.74	130 O	129 OG	156 CB	105.34
130 C	129 OG	130 CA	18.25	130 C	129 OG	152 SG	139.56
130 C	129 OG	156 N	129.77	130 C	129 OG	61 ND1	78.31
130 C	129 OG	131 OG	44.98	130 C	129 OG	131 N	13.41
130 C	129 OG	61 CG	92.64	130 C	129 OG	156 CB	119.41
130 CA	129 OG	152 SG	123.41	130 CA	129 OG	156 N	123.22
130 CA	129 OG	61 ND1	88.09	130 CA	129 OG	131 OG	59.70
130 CA	129 OG	131 N	27.14	130 CA	129 OG	61 CG	101.72
130 CA	129 OG	156 CB	122.70	152 SG	129 OG	156 N	70.43
152 SG	129 OG	61 ND1	98.33	152 SG	129 OG	131 OG	132.25

Fig. 12J

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
152 SG	129 OG	131 N	136.81	152 SG	129 OG	61 CG	87.05
152 SG	129 OG	156 CB	92.58	156 N	129 OG	61 ND1	148.19
156 N	129 OG	131 OG	154.03	156 N	129 OG	131 N	142.72
156 N	129 OG	61 CG	135.04	156 N	129 OG	156 CB	26.68
61 ND1	129 OG	131 OG	36.65	61 ND1	129 OG	131 N	64.93
61 ND1	129 OG	61 CG	14.34	61 ND1	129 OG	156 CB	132.96
131 OG	129 OG	131 N	32.77	131 OG	129 OG	61 CG	50.41
131 OG	129 OG	156 CB	127.55	131 N	129 OG	61 CG	79.24
131 N	129 OG	156 CB	128.62	61 CG	129 OG	156 CB	125.31
129 O	129 C	130 N	122.05	129 O	129 C	129 CA	119.64
129 O	129 C	129 N	94.39	129 O	129 C	130 CA	91.21
129 O	129 C	129 CB	101.89	129 O	129 C	129 OG	112.10
129 O	129 C	130 C	89.57	129 O	129 C	128 C	105.50
129 O	129 C	130 CB	103.44	129 O	129 C	130 O	105.04
129 O	129 C	131 N	72.04	129 O	129 C	128 O	122.50
129 O	129 C	321 OH2	148.65	129 O	129 C	128 CA	92.75
129 O	129 C	61 CE1	64.66	129 O	129 C	128 CB	88.97
129 O	129 C	148 O	44.70	129 O	129 C	61 NE2	73.43
129 O	129 C	128 CG2	102.76	129 O	129 C	130 CG	97.32
129 O	129 C	131 CA	76.07	129 O	129 C	131 OG	65.61
129 O	129 C	27 CD1	93.30	129 O	129 C	157 NH2	133.24
130 N	129 C	129 CA	118.07	130 N	129 C	129 N	131.85
130 N	129 C	130 CA	30.98	130 N	129 C	129 CB	129.70
130 N	129 C	129 OG	106.28	130 N	129 C	130 C	42.69
130 N	129 C	128 C	119.41	130 N	129 C	130 CB	20.77
130 N	129 C	130 O	39.01	130 N	129 C	131 N	59.98
130 N	129 C	128 O	106.95	130 N	129 C	321 OH2	89.28
130 N	129 C	128 CA	124.58	130 N	129 C	61 CE1	118.22
130 N	129 C	128 CB	112.67	130 N	129 C	148 O	77.75
130 N	129 C	61 NE2	125.86	130 N	129 C	128 CG2	96.51
130 N	129 C	130 CG	25.11	130 N	129 C	131 CA	62.61
130 N	129 C	131 OG	87.55	130 N	129 C	27 CD1	66.30
130 N	129 C	157 NH2	18.25	129 CA	129 C	129 N	36.18
129 CA	129 C	130 CA	149.05	129 CA	129 C	129 CB	34.04
129 CA	129 C	129 OG	52.24	129 CA	129 C	130 C	143.15
129 CA	129 C	128 C	33.84	129 CA	129 C	130 CB	134.31
129 CA	129 C	130 O	125.18	129 CA	129 C	131 N	151.23
129 CA	129 C	128 O	26.20	129 CA	129 C	321 OH2	29.14
129 CA	129 C	128 CA	46.33	129 CA	129 C	61 CE1	92.00
129 CA	129 C	128 CB	63.12	129 CA	129 C	148 O	164.17
129 CA	129 C	61 NE2	76.57	129 CA	129 C	128 CG2	64.81
129 CA	129 C	130 CG	141.70	129 CA	129 C	131 CA	141.03
129 CA	129 C	131 OG	123.06	129 CA	129 C	27 CD1	105.83
129 CA	129 C	157 NH2	106.21	129 N	129 C	130 CA	149.50

Fig. 12K

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 N	129 C	129 CB	58.49	129 N	129 C	129 OG	84.14
129 N	129 C	130 C	174.51	129 N	129 C	128 C	12.62
129 N	129 C	130 CB	133.57	129 N	129 C	130 O	159.81
129 N	129 C	131 N	166.36	129 N	129 C	128 O	28.26
129 N	129 C	321 OH2	59.46	129 N	129 C	128 CA	12.49
129 N	129 C	61 CE1	104.89	129 N	129 C	128 CB	31.01
129 N	129 C	148 O	133.83	129 N	129 C	61 NE2	92.00
129 N	129 C	128 CG2	41.03	129 N	129 C	130 CG	140.46
129 N	129 C	131 CA	165.35	129 N	129 C	131 OG	139.14
129 N	129 C	27 CD1	82.69	129 N	129 C	157 NH2	130.53
130 CA	129 C	129 CB	148.63	130 CA	129 C	129 OG	121.17
130 CA	129 C	130 C	26.26	130 CA	129 C	128 C	140.61
130 CA	129 C	130 CB	17.88	130 CA	129 C	130 O	37.70
130 CA	129 C	131 N	36.42	130 CA	129 C	128 O	134.02
130 CA	129 C	321 OH2	120.12	130 CA	129 C	128 CA	137.41
130 CA	129 C	61 CE1	104.60	130 CA	129 C	128 CB	119.45
130 CA	129 C	148 O	46.77	130 CA	129 C	61 NE2	118.29
130 CA	129 C	128 CG2	108.53	130 CA	129 C	130 CG	9.92
130 CA	129 C	131 CA	43.61	130 CA	129 C	131 OG	69.75
130 CA	129 C	27 CD1	67.05	130 CA	129 C	157 NH2	44.16
129 CB	129 C	129 OG	27.48	129 CB	129 C	130 C	124.35
129 CB	129 C	128 C	62.82	129 CB	129 C	130 CB	150.37
129 CB	129 C	130 O	110.95	129 CB	129 C	131 N	121.78
129 CB	129 C	128 O	59.95	129 CB	129 C	321 OH2	51.08
129 CB	129 C	128 CA	70.95	129 CB	129 C	61 CE1	58.03
129 CB	129 C	128 CB	89.48	129 CB	129 C	148 O	135.70
129 CB	129 C	61 NE2	42.61	129 CB	129 C	128 CG2	96.32
129 CB	129 C	130 CG	151.73	129 CB	129 C	131 CA	112.01
129 CB	129 C	131 OG	89.75	129 CB	129 C	27 CD1	138.93
129 CB	129 C	157 NH2	111.87	129 OG	129 C	130 C	97.91
129 OG	129 C	128 C	85.60	129 OG	129 C	130 CB	125.42
129 OG	129 C	130 O	83.53	129 OG	129 C	131 N	99.41
129 OG	129 C	128 O	77.17	129 OG	129 C	321 OH2	52.83
129 OG	129 C	128 CA	96.22	129 OG	129 C	61 CE1	50.88
129 OG	129 C	128 CB	114.38	129 OG	129 C	148 O	125.73
129 OG	129 C	61 NE2	39.02	129 OG	129 C	128 CG2	116.72
129 OG	129 C	130 CG	124.87	129 OG	129 C	131 CA	89.15
129 OG	129 C	131 OG	72.66	129 OG	129 C	27 CD1	152.16
129 OG	129 C	157 NH2	88.05	130 C	129 C	128 C	162.05
130 C	129 C	130 CB	41.42	130 C	129 C	130 O	18.01
130 C	129 C	131 N	18.27	130 C	129 C	128 O	147.28
130 C	129 C	321 OH2	117.87	130 C	129 C	128 CA	163.63
130 C	129 C	61 CE1	80.24	130 C	129 C	128 CB	145.61
130 C	129 C	148 O	48.45	130 C	129 C	61 NE2	92.77

Fig. 12L

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 C	129 C	128 CG2	134.23	130 C	129 C	130 CG	34.83
130 C	129 C	131 CA	20.13	130 C	129 C	131 OG	46.22
130 C	129 C	27 CD1	93.31	130 C	129 C	157 NH2	44.77
128 C	129 C	130 CB	123.32	128 C	129 C	130 O	149.46
128 C	129 C	131 N	174.93	128 C	129 C	128 O	17.21
128 C	129 C	321 OH2	51.24	128 C	129 C	128 CA	14.19
128 C	129 C	61 CE1	114.79	128 C	129 C	128 CB	29.29
128 C	129 C	148 O	140.66	128 C	129 C	61 NE2	100.76
128 C	129 C	128 CG2	33.62	128 C	129 C	130 CG	130.87
128 C	129 C	131 CA	174.74	128 C	129 C	131 OG	149.64
128 C	129 C	27 CD1	76.43	128 C	129 C	157 NH2	118.22
130 CB	129 C	130 O	47.15	130 CB	129 C	131 N	54.09
130 CB	129 C	128 O	116.23	130 CB	129 C	321 OH2	107.26
130 CB	129 C	128 CA	122.53	130 CB	129 C	61 CE1	121.52
130 CB	129 C	128 CB	106.04	130 CB	129 C	148 O	61.13
130 CB	129 C	61 NE2	134.03	130 CB	129 C	128 CG2	92.86
130 CB	129 C	130 CG	8.06	130 CB	129 C	131 CA	60.49
130 CB	129 C	131 OG	86.90	130 CB	129 C	27 CD1	54.16
130 CB	129 C	157 NH2	38.51	130 O	129 C	131 N	33.24
130 O	129 C	128 O	132.41	130 O	129 C	321 OH2	100.38
130 O	129 C	128 CA	160.95	130 O	129 C	61 CE1	79.25
130 O	129 C	128 CB	151.59	130 O	129 C	148 O	66.19
130 O	129 C	61 NE2	88.41	130 O	129 C	128 CG2	135.46
130 O	129 C	130 CG	43.16	130 O	129 C	131 CA	29.52
130 O	129 C	131 OG	50.02	130 O	129 C	27 CD1	101.28
130 O	129 C	157 NH2	33.12	131 N	129 C	128 O	165.39
131 N	129 C	321 OH2	132.77	131 N	129 C	128 CA	161.39
131 N	129 C	61 CE1	68.47	131 N	129 C	128 CB	145.65
131 N	129 C	148 O	34.84	131 N	129 C	61 NE2	82.90
131 N	129 C	128 CG2	141.90	131 N	129 C	130 CG	46.31
131 N	129 C	131 CA	10.26	131 N	129 C	131 OG	33.71
131 N	129 C	27 CD1	99.15	131 N	129 C	157 NH2	62.99
128 O	129 C	321 OH2	34.87	128 O	129 C	128 CA	31.00
128 O	129 C	61 CE1	117.33	128 O	129 C	128 CB	42.38
128 O	129 C	148 O	155.18	128 O	129 C	61 NE2	102.00
128 O	129 C	128 CG2	39.59	128 O	129 C	130 CG	124.29
128 O	129 C	131 CA	159.99	128 O	129 C	131 OG	149.21
128 O	129 C	27 CD1	79.64	128 O	129 C	157 NH2	102.52
321 OH2	129 C	128 CA	65.42	321 OH2	129 C	61 CE1	103.19
321 OH2	129 C	128 CB	76.75	321 OH2	129 C	148 O	166.01
321 OH2	129 C	61 NE2	89.41	321 OH2	129 C	128 CG2	69.83
321 OH2	129 C	130 CG	113.82	321 OH2	129 C	131 CA	125.23
321 OH2	129 C	131 OG	121.79	321 OH2	129 C	27 CD1	99.47
321 OH2	129 C	157 NH2	77.18	128 CA	129 C	61 CE1	115.33

Fig. 12M

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 CA	129 C	128 CB	18.53	128 CA	129 C	148 O	126.57
128 CA	129 C	61 NE2	103.43	128 CA	129 C	128 CG2	29.70
128 CA	129 C	130 CG	128.85	128 CA	129 C	131 CA	168.77
128 CA	129 C	131 OG	147.85	128 CA	129 C	27 CD1	70.39
128 CA	129 C	157 NH2	127.90	61 CE1	129 C	128 CB	129.11
61 CE1	129 C	148 O	78.89	61 CE1	129 C	61 NE2	15.43
61 CE1	129 C	128 CG2	144.82	61 CE1	129 C	130 CG	114.27
61 CE1	129 C	131 CA	61.10	61 CE1	129 C	131 OG	34.86
61 CE1	129 C	27 CD1	156.87	61 CE1	129 C	157 NH2	107.32
128 CB	129 C	148 O	112.95	128 CB	129 C	61 NE2	119.56
128 CB	129 C	128 CG2	17.06	128 CB	129 C	130 CG	111.56
128 CB	129 C	131 CA	155.75	128 CB	129 C	131 OG	153.81
128 CB	129 C	27 CD1	52.51	128 CB	129 C	157 NH2	121.62
148 O	129 C	61 NE2	93.93	148 O	129 C	128 CG2	116.42
148 O	129 C	130 CG	53.97	148 O	129 C	131 CA	43.54
148 O	129 C	131 OG	53.23	148 O	129 C	27 CD1	80.26
148 O	129 C	157 NH2	88.96	61 NE2	129 C	128 CG2	133.00
61 NE2	129 C	130 CG	127.54	61 NE2	129 C	131 CA	74.74
61 NE2	129 C	131 OG	49.21	61 NE2	129 C	27 CD1	165.36
61 NE2	129 C	157 NH2	111.37	128 CG2	129 C	130 CG	99.46
128 CG2	129 C	131 CA	151.39	128 CG2	129 C	131 OG	167.88
128 CG2	129 C	27 CD1	42.81	128 CG2	129 C	157 NH2	104.56
130 CG	129 C	131 CA	53.18	130 CG	129 C	131 OG	79.47
130 CG	129 C	27 CD1	59.09	130 CG	129 C	157 NH2	41.21
131 CA	129 C	131 OG	26.43	131 CA	129 C	27 CD1	108.62
131 CA	129 C	157 NH2	61.95	131 OG	129 C	27 CD1	131.08
131 OG	129 C	157 NH2	82.70	27 CD1	129 C	157 NH2	82.12
129 C	129 O	130 N	30.35	129 C	129 O	129 CA	33.87
129 C	129 O	129 N	59.08	129 C	129 O	130 CA	62.27
129 C	129 O	129 CB	54.82	129 C	129 O	130 C	69.65
129 C	129 O	129 OG	49.93	129 C	129 O	131 N	89.72
129 C	129 O	128 C	57.43	129 C	129 O	148 O	123.10
129 C	129 O	130 CB	59.77	129 C	129 O	130 O	58.75
129 C	129 O	61 CE1	100.53	129 C	129 O	148 C	137.13
129 C	129 O	61 NE2	92.31	129 C	129 O	128 O	45.06
129 C	129 O	128 CA	72.67	129 C	129 O	131 OG	101.33
129 C	129 O	131 CA	90.06	129 C	129 O	128 CB	76.78
129 C	129 O	148 ND1	151.06	129 C	129 O	61 ND1	112.00
129 C	129 O	131 CB	103.03	129 C	129 O	148 CE1	138.86
129 C	129 O	130 CG	69.65	129 C	129 O	128 CG2	64.49
130 N	129 O	129 CA	64.13	130 N	129 O	129 N	85.39
130 N	129 O	130 CA	32.00	130 N	129 O	129 CB	82.83
130 N	129 O	130 C	44.51	130 N	129 O	129 OG	71.39
130 N	129 O	131 N	65.15	130 N	129 O	128 C	82.26

Fig. 12N

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
130 N	129 O	148 O	93.03	130 N	129 O	130 CB	30.20
130 N	129 O	130 O	38.28	130 N	129 O	61 CE1	108.49
130 N	129 O	148 C	106.82	130 N	129 O	61 NE2	107.74
130 N	129 O	128 O	71.27	130 N	129 O	128 CA	94.63
130 N	129 O	131 OG	90.09	130 N	129 O	131 CA	68.90
130 N	129 O	128 CB	91.19	130 N	129 O	148 ND1	131.56
130 N	129 O	61 ND1	117.45	130 N	129 O	131 CB	84.84
130 N	129 O	148 CE1	127.33	130 N	129 O	130 CG	39.45
130 N	129 O	128 CG2	75.85	129 CA	129 O	129 N	31.67
129 CA	129 O	130 CA	96.12	129 CA	129 O	129 CB	29.81
129 CA	129 O	130 C	100.96	129 CA	129 O	129 OG	40.52
129 CA	129 O	131 N	118.95	129 CA	129 O	128 C	33.00
129 CA	129 O	148 O	156.88	129 CA	129 O	130 CB	92.60
129 CA	129 O	130 O	88.24	129 CA	129 O	61 CE1	91.63
129 CA	129 O	148 C	170.88	129 CA	129 O	61 NE2	77.52
129 CA	129 O	128 O	22.12	129 CA	129 O	128 CA	49.00
129 CA	129 O	131 OG	113.50	129 CA	129 O	131 CA	115.84
129 CA	129 O	128 CB	61.46	129 CA	129 O	148 ND1	148.47
129 CA	129 O	61 ND1	102.07	129 CA	129 O	131 CB	122.93
129 CA	129 O	148 CE1	135.17	129 CA	129 O	130 CG	103.01
129 CA	129 O	128 CG2	56.96	129 N	129 O	130 CA	114.74
129 N	129 O	129 CB	48.68	129 N	129 O	130 C	128.60
129 N	129 O	129 OG	67.49	129 N	129 O	131 N	148.77
129 N	129 O	128 C	5.43	129 N	129 O	148 O	159.15
129 N	129 O	130 CB	106.36	129 N	129 O	130 O	117.61
129 N	129 O	61 CE1	107.68	129 N	129 O	148 C	151.98
129 N	129 O	61 NE2	91.86	129 N	129 O	128 O	14.24
129 N	129 O	128 CA	17.66	129 N	129 O	131 OG	140.56
129 N	129 O	131 CA	147.34	129 N	129 O	128 CB	33.20
129 N	129 O	148 ND1	142.23	129 N	129 O	61 ND1	114.34
129 N	129 O	131 CB	153.27	129 N	129 O	148 CE1	138.98
129 N	129 O	130 CG	117.16	129 N	129 O	128 CG2	36.05
130 CA	129 O	129 CB	111.50	130 CA	129 O	130 C	24.98
130 CA	129 O	129 OG	94.87	130 CA	129 O	131 N	40.78
130 CA	129 O	128 C	110.63	130 CA	129 O	148 O	61.05
130 CA	129 O	130 CB	11.79	130 CA	129 O	130 O	31.00
130 CA	129 O	61 CE1	108.61	130 CA	129 O	148 C	74.86
130 CA	129 O	61 NE2	116.78	130 CA	129 O	128 O	101.31
130 CA	129 O	128 CA	119.02	130 CA	129 O	131 OG	75.71
130 CA	129 O	131 CA	48.35	130 CA	129 O	128 CB	108.49
130 CA	129 O	148 ND1	103.00	130 CA	129 O	61 ND1	111.87
130 CA	129 O	131 CB	64.47	130 CA	129 O	148 CE1	104.06
130 CA	129 O	130 CG	10.27	130 CA	129 O	128 CG2	93.66
129 CB	129 O	130 C	103.90	129 CB	129 O	129 OG	21.65

Fig. 120

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129 CB	129 O	131 N	113.82	129 CB	129 O	128 C	52.87
129 CB	129 O	148 O	151.76	129 CB	129 O	130 CB	112.97
129 CB	129 O	130 O	90.28	129 CB	129 O	61 CE1	62.88
129 CB	129 O	148 C	155.41	129 CB	129 O	61 NE2	48.03
129 CB	129 O	128 O	47.12	129 CB	129 O	128 CA	64.90
129 CB	129 O	131 OG	91.88	129 CB	129 O	131 CA	106.28
129 CB	129 O	128 CB	81.83	129 CB	129 O	148 ND1	118.69
129 CB	129 O	61 ND1	72.68	129 CB	129 O	131 CB	105.34
129 CB	129 O	148 CE1	105.50	129 CB	129 O	130 CG	121.05
129 CB	129 O	128 CG2	82.65	130 C	129 O	129 OG	83.13
130 C	129 O	131 N	20.72	130 C	129 O	128 C	126.24
130 C	129 O	148 O	56.99	130 C	129 O	130 CB	36.76
130 C	129 O	130 O	13.74	130 C	129 O	61 CE1	83.91
130 C	129 O	148 C	71.44	130 C	129 O	61 NE2	93.63
130 C	129 O	128 O	114.40	130 C	129 O	128 CA	139.10
130 C	129 O	131 OG	51.17	130 C	129 O	131 CA	25.19
130 C	129 O	128 CB	132.37	130 C	129 O	148 ND1	87.12
130 C	129 O	61 ND1	86.91	130 C	129 O	131 CB	41.68
130 C	129 O	148 CE1	83.81	130 C	129 O	130 CG	31.86
130 C	129 O	128 CG2	117.00	129 OG	129 O	131 N	92.19
129 OG	129 O	128 C	70.77	129 OG	129 O	148 O	131.52
129 OG	129 O	130 CB	99.52	129 OG	129 O	130 O	69.82
129 OG	129 O	61 CE1	53.56	129 OG	129 O	148 C	139.99
129 OG	129 O	61 NE2	42.66	129 OG	129 O	128 O	62.06
129 OG	129 O	128 CA	84.73	129 OG	129 O	131 OG	73.94
129 OG	129 O	131 CA	84.90	129 OG	129 O	128 CB	100.33
129 OG	129 O	148 ND1	112.13	129 OG	129 O	61 ND1	64.97
129 OG	129 O	131 CB	85.82	129 OG	129 O	148 CE1	97.46
129 OG	129 O	130 CG	105.07	129 OG	129 O	128 CG2	97.47
131 N	129 O	128 C	146.86	131 N	129 O	148 O	41.37
131 N	129 O	130 CB	51.90	131 N	129 O	130 O	31.20
131 N	129 O	61 CE1	74.46	131 N	129 O	148 C	54.71
131 N	129 O	61 NE2	87.77	131 N	129 O	128 O	134.75
131 N	129 O	128 CA	159.35	131 N	129 O	131 OG	37.22
131 N	129 O	131 CA	9.83	131 N	129 O	128 CB	148.16
131 N	129 O	148 ND1	66.43	131 N	129 O	61 ND1	73.93
131 N	129 O	131 CB	23.97	131 N	129 O	148 CE1	64.07
131 N	129 O	130 CG	43.35	131 N	129 O	128 CG2	134.19
128 C	129 O	148 O	154.38	128 C	129 O	130 CB	101.77
128 C	129 O	130 O	116.18	128 C	129 O	61 CE1	112.86
128 C	129 O	148 C	149.18	128 C	129 O	61 NE2	97.03
128 C	129 O	128 O	12.59	128 C	129 O	128 CA	16.27
128 C	129 O	131 OG	144.52	128 C	129 O	131 CA	147.12
128 C	129 O	128 CB	29.56	128 C	129 O	148 ND1	145.97

Fig. 12P

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 C	129 O	61 ND1	119.73	128 C	129 O	131 CB	155.87
128 C	129 O	148 CE1	144.01	128 C	129 O	130 CG	112.45
128 C	129 O	128 CG2	30.91	148 O	129 O	130 CB	65.75
148 O	129 O	130 O	70.32	148 O	129 O	61 CE1	92.56
148 O	129 O	148 C	14.61	148 O	129 O	61 NE2	108.34
148 O	129 O	128 O	155.67	148 O	129 O	128 CA	143.33
148 O	129 O	131 OG	60.10	148 O	129 O	131 CA	47.14
148 O	129 O	128 CB	126.30	148 O	129 O	148 ND1	46.78
148 O	129 O	61 ND1	84.83	148 O	129 O	131 CB	46.42
148 O	129 O	148 CE1	55.64	148 O	129 O	130 CG	54.94
148 O	129 O	128 CG2	123.54	130 CB	129 O	130 O	41.54
130 CB	129 O	61 CE1	120.07	130 CB	129 O	148 C	78.29
130 CB	129 O	61 NE2	127.05	130 CB	129 O	128 O	93.83
130 CB	129 O	128 CA	108.42	130 CB	129 O	131 OG	87.45
130 CB	129 O	131 CA	59.90	130 CB	129 O	128 CB	96.91
130 CB	129 O	148 ND1	110.71	130 CB	129 O	61 ND1	123.66
130 CB	129 O	131 CB	75.80	130 CB	129 O	148 CE1	113.86
130 CB	129 O	130 CG	11.00	130 CB	129 O	128 CG2	82.32
130 O	129 O	61 CE1	78.95	130 O	129 O	148 C	84.60
130 O	129 O	61 NE2	85.81	130 O	129 O	128 O	103.78
130 O	129 O	128 CA	130.97	130 O	129 O	131 OG	52.22
130 O	129 O	131 CA	31.78	130 O	129 O	128 CB	129.45
130 O	129 O	148 ND1	95.34	130 O	129 O	61 ND1	84.44
130 O	129 O	131 CB	46.88	130 O	129 O	148 CE1	89.14
130 O	129 O	130 CG	40.26	130 O	129 O	128 CG2	114.05
61 CE1	129 O	148 C	92.53	61 CE1	129 O	61 NE2	15.83
61 CE1	129 O	128 O	109.78	61 CE1	129 O	128 CA	118.54
61 CE1	129 O	131 OG	37.82	61 CE1	129 O	131 CA	64.76
61 CE1	129 O	128 CB	135.90	61 CE1	129 O	148 ND1	58.66
61 CE1	129 O	61 ND1	11.58	61 CE1	129 O	131 CB	52.85
61 CE1	129 O	148 CE1	44.12	61 CE1	129 O	130 CG	115.48
61 CE1	129 O	128 CG2	143.74	148 C	129 O	61 NE2	107.50
148 C	129 O	128 O	157.19	148 C	129 O	128 CA	134.35
148 C	129 O	131 OG	66.06	148 C	129 O	131 CA	59.12
148 C	129 O	128 CB	119.65	148 C	129 O	148 ND1	38.53
148 C	129 O	61 ND1	82.88	148 C	129 O	131 CB	54.64
148 C	129 O	148 CE1	50.53	148 C	129 O	130 CG	67.86
148 C	129 O	128 CG2	121.35	61 NE2	129 O	128 O	94.38
61 NE2	129 O	128 CA	103.28	61 NE2	129 O	131 OG	52.49
61 NE2	129 O	131 CA	77.94	61 NE2	129 O	128 CB	121.00
61 NE2	129 O	148 ND1	71.54	61 NE2	129 O	61 ND1	24.65
61 NE2	129 O	131 CB	67.71	61 NE2	129 O	148 CE1	57.65
61 NE2	129 O	130 CG	125.35	61 NE2	129 O	128 CG2	127.91
128 O	129 O	128 CA	28.69	128 O	129 O	131 OG	135.60

Fig. 12Q

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
128 O	129 O	131 CA	134.53	128 O	129 O	128 CB	39.38
128 O	129 O	148 ND1	155.45	128 O	129 O	61 ND1	118.67
128 O	129 O	131 CB	144.43	128 O	129 O	148 CE1	148.64
128 O	129 O	130 CG	104.81	128 O	129 O	128 CG2	35.86
128 CA	129 O	131 OG	155.40	128 CA	129 O	131 CA	162.69
128 CA	129 O	128 CB	17.97	128 CA	129 O	148 ND1	133.46
128 CA	129 O	61 ND1	122.22	128 CA	129 O	131 CB	170.17
128 CA	129 O	148 CE1	136.57	128 CA	129 O	130 CG	117.95
128 CA	129 O	128 CG2	27.49	131 OG	129 O	131 CA	27.97
131 OG	129 O	128 CB	173.37	131 OG	129 O	148 ND1	49.75
131 OG	129 O	61 ND1	36.82	131 OG	129 O	131 CB	15.23
131 OG	129 O	148 CE1	38.90	131 OG	129 O	130 CG	80.14
131 OG	129 O	128 CG2	165.42	131 CA	129 O	128 CB	156.81
131 CA	129 O	148 ND1	63.60	131 CA	129 O	61 ND1	64.79
131 CA	129 O	131 CB	16.50	131 CA	129 O	148 CE1	58.76
131 CA	129 O	130 CG	52.18	131 CA	129 O	128 CG2	141.88
128 CB	129 O	148 ND1	132.06	128 CB	129 O	61 ND1	137.85
128 CB	129 O	131 CB	171.25	128 CB	129 O	148 CE1	141.13
128 CB	129 O	130 CG	104.86	128 CB	129 O	128 CG2	15.55
148 ND1	129 O	61 ND1	47.49	148 ND1	129 O	131 CB	48.98
148 ND1	129 O	148 CE1	14.72	148 ND1	129 O	130 CG	99.73
148 ND1	129 O	128 CG2	144.22	61 ND1	129 O	131 CB	50.53
61 ND1	129 O	148 CE1	33.20	61 ND1	129 O	130 CG	116.95
61 ND1	129 O	128 CG2	149.41	131 CB	129 O	148 CE1	42.54
131 CB	129 O	130 CG	67.27	131 CB	129 O	128 CG2	158.12
148 CE1	129 O	130 CG	103.40	148 CE1	129 O	128 CG2	155.68
130 CG	129 O	128 CG2	91.07				

Fig. 13A

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
129OG	61CD2	129CB	19.02	129OG	61CD2	129O	43.06
129CB	61CD2	129O	37.16	148CE1	61CD2	129O	78.30
148CE1	61ND1	131CB	52.38	148CE1	61ND1	148NE2	14.31
129OG	61ND1	131CB	82.11	131CB	61ND1	148NE2	45.16
129OG	61CE1	129CB	17.72	129OG	61CE1	129O	49.00
129OG	61CE1	129C	37.16	129OG	61CE1	131CA	87.97
129OG	61CE1	131N	76.81	129CB	61CE1	129O	39.96
129CB	61CE1	129C	32.01	129CB	61CE1	131CA	93.51
129CB	61CE1	131N	79.08	129O	61CE1	131CB	74.23
129O	61CE1	148CE1	82.40	129O	61CE1	129C	13.37
129O	61CE1	131CA	63.73	129O	61CE1	131N	46.91
131CB	61CE1	148CE1	53.06	131CB	61CE1	129C	77.45
131CB	61CE1	131CA	17.24	131CB	61CE1	131N	29.58
148CE1	61CE1	129C	94.62	148CE1	61CE1	131CA	67.27
148CE1	61CE1	131N	68.05	129C	61CE1	131CA	63.93
129C	61CE1	131N	48.10	131CA	61CE1	131N	16.86
129OG	61NE2	129CB	25.02	129OG	61NE2	129O	58.32
129OG	61NE2	129C	43.65	129OG	61NE2	129CA	30.38
129CB	61NE2	129O	48.45	129CB	61NE2	129C	36.82
129CB	61NE2	129CA	16.19	129O	61NE2	129C	14.73
129O	61NE2	129CA	32.61	129O	61NE2	148CE1	86.57
129C	61NE2	129CA	20.67	129C	61NE2	148CE1	99.19
61NE2	129CA	152SG	77.41	61NE2	129CB	61CE1	16.25
61NE2	129CB	61CD2	14.16	152SG	129CB	61CD2	91.44
61CE1	129CB	61CD2	29.75	61NE2	129OG	61CE1	23.54
61NE2	129OG	61CD2	10.38	61NE2	129OG	61ND1	22.43
61NE2	129OG	152SG	91.43	61NE2	129OG	61CG	11.68
61CE1	129OG	61CD2	31.62	61CE1	129OG	61ND1	6.87
61CE1	129OG	61CG	20.09	61CD2	129OG	61ND1	28.57
61CD2	129OG	152SG	81.45	61CD2	129OG	61CG	13.41
61ND1	129OG	61CG	15.68	156CG	129OG	152SG	89.53
152SG	129OG	61CG	91.59	131N	129C	61NE2	82.32
131N	129C	148O	36.39	131N	129C	61CE1	69.68
61NE2	129C	148O	83.14	61NE2	129C	61CE1	15.62
148O	129C	61CE1	78.52	61NE2	129O	131N	93.33
61NE2	129O	61CE1	16.99	61NE2	129O	61CD2	13.22
61NE2	129O	131CA	81.79	131N	129O	148O	42.21
131N	129O	61CE1	77.02	131N	129O	148C	55.96
131N	129O	131CA	11.75	148O	129O	61CE1	93.27
148O	129O	148C	13.81	148O	129O	61CD2	99.88
148O	129O	131CA	48.34	61CE1	129O	148C	97.42
61CE1	129O	61CD2	28.11	61CE1	129O	131CA	65.34
148C	129O	61CD2	97.33	148C	129O	131CA	61.48
61CD2	129O	131CA	89.15	148O	131N	129O	69.99

Fig. 13B

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>
148O	131N	148C	2.84	148O	131N	129C	83.60
148O	131N	148N	36.71	148O	131N	148CA	19.19
148O	131N	61CE1	94.32	129O	131N	148C	72.41
129O	131N	129C	16.68	129O	131N	148CA	88.32
129O	131N	157NH2	88.88	129O	131N	61CE1	56.08
148C	131N	129C	86.23	148C	131N	148N	34.08
148C	131N	148CA	16.44	148C	131N	61CE1	94.65
129C	131N	157NH2	72.38	129C	131N	61CE1	62.21
148N	131N	148CA	17.83	157NH2	131N	61CE1	96.41
148O	131CA	148N	36.27	148O	131CA	148C	7.03
148O	131CA	129O	49.93	148O	131CA	61CE1	83.50
148N	131CA	148C	30.32	148N	131CA	129O	85.91
148C	131CA	129O	55.59	148C	131CA	61CE1	84.67
129O	131CA	61CE1	50.93	148NE2	131CB	148O	78.60
148NE2	131CB	148CD2	20.18	148NE2	131CB	148CE1	19.26
148NE2	131CB	61CE1	81.78	148NE2	131CB	148ND1	29.14
148NE2	131CB	148CG	29.92	148NE2	131CB	148N	65.64
148NE2	131CB	148C	67.71	148NE2	131CB	61ND1	69.90
148O	131CB	148CD2	66.42	148O	131CB	148CE1	69.14
148O	131CB	61CE1	92.06	148O	131CB	148ND1	52.14
148O	131CB	148CG	49.88	148O	131CB	148N	38.61
148O	131CB	148C	11.51	148O	131CB	61ND1	99.72
148CD2	131CB	148CE1	31.89	148CD2	131CB	61CE1	98.25
148CD2	131CB	148ND1	29.69	148CD2	131CB	148CG	17.70
148CD2	131CB	148N	46.03	148CD2	131CB	148C	54.91
148CD2	131CB	61ND1	88.41	148CE1	131CB	61CE1	66.36
148CE1	131CB	148ND1	17.33	148CE1	131CB	148CG	29.95
148CE1	131CB	148N	69.27	148CE1	131CB	148C	60.00
148CE1	131CB	61ND1	57.48	61CE1	131CB	148ND1	73.80
61CE1	131CB	148CG	91.81	61CE1	131CB	148C	93.93
61CE1	131CB	61ND1	16.02	148ND1	131CB	148CG	18.02
148ND1	131CB	148N	54.81	148ND1	131CB	148C	42.69
148ND1	131CB	61ND1	68.89	148CG	131CB	148N	39.36
148CG	131CB	148C	38.54	148CG	131CB	61ND1	86.14
148N	131CB	148C	31.66	148C	131CB	61ND1	98.62
148O	131C	148N	37.37	148N	131O	148O	44.95
148N	131O	148C	32.33	148N	131O	148CA	13.20
148O	131O	148C	12.85	148O	131O	148CA	31.80
148C	131O	148CA	19.13	131O	148N	131C	11.83
131O	148N	131CB	44.24	131O	148N	131N	38.86
131O	148N	131CA	29.72	131C	148N	131CB	32.41
131C	148N	131N	32.25	131C	148N	131CA	19.13
131CB	148N	131N	32.34	131CB	148N	131CA	18.99
131N	148N	131CA	18.15	131O	148CA	131N	34.00

Fig. 13C

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>
131CB	148CE1	61ND1	70.14	131CB	148CE1	61CG	87.74
131CB	148CE1	61CE1	60.59	131CB	148CE1	61CD2	87.10
131CB	148CE1	61NE2	71.26	61ND1	148CE1	61CG	18.52
61ND1	148CE1	61CE1	16.74	61ND1	148CE1	61CD2	28.08
61ND1	148CE1	61CB	32.50	61ND1	148CE1	61CA	49.71
61ND1	148CE1	61NE2	26.67	61CG	148CE1	61CE1	28.54
61CG	148CE1	61CD2	17.02	61CG	148CE1	61CB	18.75
61CG	148CE1	61CA	32.50	61CG	148CE1	61NE2	27.41
61CE1	148CE1	61CD2	27.52	61CE1	148CE1	61CB	46.34
61CE1	148CE1	61CA	60.86	61CE1	148CE1	61NE2	16.00
61CD2	148CE1	61CB	32.66	61CD2	148CE1	61CA	39.09
61CD2	148CE1	61NE2	16.68	61CB	148CE1	61CA	18.92
61CB	148CE1	61NE2	45.92	61CA	148CE1	61NE2	55.42
131CB	148NE2	61ND1	64.94	131N	148C	129O	51.62
131N	148C	131O	36.94	131N	148C	131CB	31.72
131N	148C	131CA	15.22	129O	148C	131O	88.46
129O	148C	131CB	68.45	129O	148C	131CA	62.93
131O	148C	131CB	38.96	131O	148C	131CA	29.36
131CB	148C	131CA	18.33	131N	148O	131CA	19.47
131N	148O	131CB	40.86	131N	148O	131O	47.43
131N	148O	129O	67.80	131N	148O	131C	32.92
131N	148O	129C	60.01	131CA	148O	131CB	23.57
131CA	148O	131O	37.54	131CA	148O	129O	81.73
131CA	148O	131C	20.95	131CA	148O	129C	76.15
131CB	148O	131O	48.60	131CB	148O	129O	86.85
131CB	148O	131C	35.24	131CB	148O	129C	85.69
131O	148O	131C	16.59	129O	148O	129C	11.83
131C	148O	129C	92.92	129CB	152SG	129N	31.00
129CB	152SG	129CA	15.62	129CB	152SG	129OG	13.31
129N	152SG	129CA	16.86	129N	152SG	129OG	44.10
129CA	152SG	129OG	27.89	157N	156N	157CA	4.31
157N	156N	157O	37.33	157N	156N	157C	22.91
157N	156N	157CB	16.22	157CA	156N	157O	33.09
157CA	156N	157C	18.77	157CA	156N	157CB	16.57
157O	156N	157C	14.65	157O	156N	157CB	41.91
157C	156N	157CB	30.44	157N	156CA	157CA	9.28
157N	156CA	157O	32.35	157N	156CA	157C	21.11
157N	156CA	157CB	10.98	157CA	156CA	157O	33.51
157CA	156CA	157C	18.98	157CA	156CA	157CB	15.89
157O	156CA	157C	15.80	157O	156CA	157CB	43.10
157C	156CA	157CB	31.92	157N	156CB	157CA	9.84
157N	156CG	129OG	91.04	157N	156C	157CA	31.55
157N	156C	157C	41.25	157N	156C	157O	44.51
157N	156C	157CB	24.42	157N	156C	157CG	43.37

Fig. 13D

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>
157CA	156C	157C	26.80	157CA	156C	157O	44.67
157CA	156C	157CB	19.42	157CA	156C	157CG	38.68
157C	156C	157O	20.88	157C	156C	157CB	43.93
157C	156C	157CG	65.27	157O	156C	157CB	57.59
157O	156C	157CG	80.41	157CB	156C	157CG	22.87
157N	156O	157CA	32.63	157N	156O	157C	43.65
157N	156O	157O	40.81	157N	156O	157CB	32.60
157N	156O	157CG	45.85	157CA	156O	157C	25.15
157CA	156O	157O	37.46	157CA	156O	157CB	14.38
157CA	156O	157CG	35.30	157C	156O	157O	17.80
157C	156O	157CB	39.53	157C	156O	157CG	60.29
157O	156O	157CB	50.62	157O	156O	157CG	71.80
157CB	156O	157CG	21.25	156C	157N	156O	28.15
156C	157N	156CA	34.99	156C	157N	156N	65.94
156C	157N	156CB	40.62	156C	157N	156CG	55.08
156O	157N	156CA	63.13	156O	157N	156N	93.80
156O	157N	156CB	64.30	156O	157N	156CG	80.42
156CA	157N	156N	31.91	156CA	157N	156CB	23.76
156CA	157N	156CG	27.51	156N	157N	156CB	45.42
156N	157N	156CG	34.38	156CB	157N	156CG	16.54
156C	157CA	156O	27.04	156C	157CA	156CA	12.72
156C	157CA	156N	32.74	156C	157CA	156CB	19.54
156O	157CA	156CA	39.76	156O	157CA	156N	59.49
156O	157CA	156CB	40.29	156CA	157CA	156N	20.36
156CA	157CA	156CB	17.01	156N	157CA	156CB	31.47
156C	157CB	156O	17.61	156C	157CB	156CA	13.56
156C	157CB	156N	29.34	156O	157CB	156CA	30.75
156O	157CB	156N	46.94	156CA	157CB	156N	17.30
156C	157CG	156O	16.90	156C	157C	156O	20.61
156C	157C	156CA	13.16	156C	157C	156N	30.83
156O	157C	156CA	32.27	156O	157C	156N	50.49
156CA	157C	156N	18.22	156C	157O	156O	17.58
156C	157O	156N	36.58	156C	157O	156CA	18.11
156O	157O	156N	52.93	156O	157O	156CA	33.44
156N	157O	156CA	19.58				

Fig. 14

	Phi $C_n-1-N_n-C_n-C$	Psi $N-CA-C-N_{n+1}$	Omega 1 $CA_n-1-C_n-1-N_n-CA_n$	Omega 2 $CA_n-C_n-N_{n+1}-CA_{n+1}$	Chi1 $N-CA-CB-CG$	Chi2 $CA-CD-CG-XD$
Ser129	-150.1	113.4	179.3	179.9	172.9	
His148	-170.5	170.8	179.1	178.0	59.3	95.0
His61	46.4	-0.4	178.5	177.3	-75.0	118.9

Fig. 15

	Phi $C_n-1-N_n-C_{An}-C$	Psi $N-CA-C-N_{n+1}$	Omega 1 $CA_{n-1}-C_n-1-N_n-CA_n$	Omega 2 $CA_n-C_n-N_{n+1}-CA_{n+1}$	Chi1 $N-CA-CB-CG$	Chi2 $CA-CD-CG-XD$
Ser129	-140.4	123.5	179.7	179.6	-175.8	
His148	-159.5	-173.0	178.9	179.0	63.6	91.6
His61	67.4	0.6	179.0	178.0	-62.0	-75.9

Fig. 16

	Phi $C_n-1-N_n-C_{An}-C$	Psi $N-CA-C-N_{n+1}$	Omega 1 $CA_n-1-C_n-1-N_n-CA_n$	Omega 2 $CA_n-C_n-N_{n+1}-CA_{n+1}$	Chi1 $N-CA-CB-CG$	Chi2 $CA-CD-CG-XD$
Ser129	-151.5	119.5	179.3	-170.5	172.9	
His61	36.3	22.0	178.5	171.9	-61.0	-150.1
His148	-170.5	170.8	179.1	177.9	59.3	95.0

Fig. 17A

CRYST1	58.7	58.7	131.0	90.00	90.00	90.00	P4 ₃ 22
Atom	Residue AA	No.	X	Y	Z	Occup'y	B Factor
ATOM 1	N	HIS 63	32.880001	14.629000	8.245000	1.00	37.16
ATOM 2	Ca	HIS 63	33.591000	14.522000	6.961000	1.00	37.70
ATOM 3	Cβ	HIS 63	32.750000	13.848000	5.900000	1.00	33.47
ATOM 4	Cγ	HIS 63	32.007000	12.649000	6.383000	1.00	33.87
ATOM 5	Cδ2	HIS 63	30.681000	12.452000	6.569000	1.00	33.18
ATOM 6	Nδ1	HIS 63	32.612999	11.434000	6.615000	1.00	32.84
ATOM 7	Cε1	HIS 63	31.691000	10.534000	6.904000	1.00	34.18
ATOM 8	NE2	HIS 63	30.510000	11.128000	6.886000	1.00	35.62
ATOM 9	C	HIS 63	34.087002	15.815000	6.320000	1.00	39.66
ATOM 10	O	HIS 63	34.634998	15.758000	5.226000	1.00	45.41
ATOM 11	N	ASP 65	36.516998	18.048000	5.389000	1.00	43.05
ATOM 12	Ca	ASP 65	37.967999	17.917000	5.469000	1.00	44.01

Fig. 17B

<u>Atom</u>	<u>Residue</u> <u>AA</u>	<u>No.</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>Occup'y</u>	<u>B Factor</u>
ATOM 13	CB	ASP 65	38.580002	17.417999	4.172000	1.00	48.74
ATOM 14	CY	ASP 65	38.945999	15.933000	4.246000	1.00	59.43
ATOM 15	Oδ1	ASP 65	39.431999	15.451000	5.316000	1.00	61.90
ATOM 16	Oδ2	ASP 65	38.706001	15.214000	3.244000	1.00	69.17
ATOM 17	C	ASP 65	38.757999	19.056000	6.036000	1.00	43.54
ATOM 18	O	ASP 65	39.959000	18.917000	6.271000	1.00	44.62
ATOM 19	N	SER 132	31.841000	7.353000	11.712000	1.00	33.66
ATOM 20	Ca	SER 132	31.664000	7.028000	10.296000	1.00	36.58
ATOM 21	Cβ	SER 132	30.868999	8.143000	9.624000	1.00	42.29
ATOM 22	Oγ	SER 132	30.243999	7.722000	8.425000	1.00	52.62
ATOM 23	C	SER 132	33.043999	6.951000	9.712000	1.00	33.26
ATOM 24	O	SER 132	33.858002	7.819000	9.936000	1.00	36.06
ATOM 25	N	SER 134	35.426998	6.727000	6.434000	1.00	43.43

Fig. 17C

Atom	Residue AA	No.	X	Y	Z	Occup'y	B Factor
ATOM 26	C α	SER 134	35.398998	7.060000	5.004000	1.00	45.24
ATOM 27	C β	SER 134	35.264000	8.566000	4.788000	1.00	45.50
ATOM 28	O γ	SER 134	36.527000	9.208000	4.914000	1.00	47.60
ATOM 29	C	SER 134	36.659000	6.527000	4.298000	1.00	46.95
ATOM 30	O	SER 134	37.787998	6.762000	4.753000	1.00	44.83
ATOM 31	N	HIS 157	39.505001	8.498000	6.198000	1.00	39.55
ATOM 32	C α	HIS 157	39.470001	9.159000	7.516000	1.00	37.74
ATOM 33	C β	HIS 157	39.282001	10.681000	7.348000	1.00	36.93
ATOM 34	C γ	HIS 157	37.972000	11.068000	6.714000	1.00	37.30
ATOM 35	C δ 2	HIS 157	36.688999	10.772000	7.049000	1.00	34.05
ATOM 36	N δ 1	HIS 157	37.898998	11.835000	5.574000	1.00	36.80
ATOM 37	C ϵ 1	HIS 157	36.636002	11.989000	5.228000	1.00	32.40
ATOM 38	N ϵ 2	HIS 157	35.882999	11.352000	6.105000	1.00	30.28

Fig. 17D

Atom	Residue AA	No.	X	Y	Z	Occup'y	B Factor
ATOM 39 C	HIS	157	38.316002	8.662000	8.365000	1.00	36.07
ATOM 40 O	HIS	157	37.532001	7.827000	7.909000	1.00	38.95
ATOM 41 N	CYS	161	29.908001	12.239000	13.796000	1.00	23.63
ATOM 42 Ca	CYS	161	28.625999	12.628000	13.235000	1.00	26.97
ATOM 43 CB	CYS	161	28.229000	11.594000	12.179000	1.00	30.92
ATOM 44 SY	CYS	161	29.539000	10.997000	11.202000	1.00	37.06
ATOM 45 C	CYS	161	27.500999	12.689000	14.261000	1.00	26.94
ATOM 46 O	CYS	161	27.638000	12.164000	15.366000	1.00	31.09
ATOM 47 N	ARG	165	25.921000	5.944000	10.186000	1.00	38.28
ATOM 48 Ca	ARG	165	24.966999	5.345000	9.241000	1.00	41.26
ATOM 49 CB	ARG	165	25.389999	5.613000	7.786000	1.00	42.30
ATOM 50 C	ARG	165	24.823999	3.847000	9.510000	1.00	42.27
ATOM 51 O	ARG	165	23.714001	3.300000	9.536000	1.00	46.30

Fig. 17E

Atom	Residue AA	No.	X	Y	Z	Occup'y	B Factor
ATOM 52	N	ARG 166	25.959000	3.176000	9.654000	1.00	42.55
ATOM 53	C α	ARG 166	25.969999	1.760000	9.964000	1.00	42.91
ATOM 54	C β	ARG 166	27.375000	1.214000	9.766000	1.00	47.77
ATOM 55	C γ	ARG 166	27.632999	0.619000	8.402000	1.00	54.62
ATOM 56	C δ	ARG 166	29.046000	0.078000	8.317000	1.00	60.07
ATOM 57	N ϵ	ARG 166	30.000000	1.185000	8.308000	1.00	66.48
ATOM 58	C ζ	ARG 166	30.875000	1.403000	7.318000	1.00	72.12
ATOM 59	NH1	ARG 166	31.709000	2.447000	7.369000	1.00	73.13
ATOM 60	NH2	ARG 166	30.945000	0.557000	6.277000	1.00	75.29
ATOM 61	C	ARG 166	25.583000	1.743000	11.440000	1.00	42.23
ATOM 62	O	ARG 166	25.955999	2.643000	12.192000	1.00	42.86
ATOM 63	O	H ₂ O 336	31.416000	3.648000	9.731000	1.00	29.21
ATOM 64	ORGN	0.000000	0.000000	0.000000	0.000000		

Fig. 18A

ATOM 1	ATOM 2	DISTANCE BETWEEN (°A)	ATOM 1	ATOM 2	DISTANCE BETWEEN (°A)
63 N	157 Ne2	4.8	63 Ce1	132 O	4.5
63 Ca	157 Ne2	4.0	63 Ce1	132 C	4.8
63 Ca	157 Ce1	4.3	63 Ce1	161 Sy	4.9
63 Ca	65 N	4.8			
63 Ca	157 Cd2	4.9	63 Ne2	132 Oy	3.3
63 CB	157 Ne2	4.1	63 Ne2	132 CB	4.6
63 CB	157 Ce1	4.4	63 Ne2	161 Sy	4.4
63 Cy	157 Ne2	4.0	63 C	65 N	3.4
63 Cy	157 Ce1	4.7	63 C	65 Ca	4.5
63 Cd2	132 Oy	4.5	63 C	157 Ce1	4.7
63 Nd1	157 Ne2	3.2	63 C	157 Ne2	4.8
63 Nd1	157 Cy2	4.2	63 O	65 N	2.9
63 Nd1	157 Ce1	4.2	63 O	65 Ca	4.0
63 Nd1	134 CB	4.3	63 O	157 Ce1	4.3
63 Nd1	132 Oy	4.2	63 O	65 CB	4.4
			63 O	65 Cy	4.4
63 Nd1	134Oy	4.8	63 O	65 Cd2	4.7
63 Ce1	132Oy	3.0	63 O	157 Ne2	4.7
63 Ce1	132 CB	4.4	63 O	65 Od1	4.7
63 Ce1	157 Ne2	4.3	65 Cy	157 Nd1	4.4
63 Ce1	134 CB	4.6	65 Cy	157 Ce1	4.8

Fig. 18B

ATOM 1	ATOM 2	DISTANCE BETWEEN (°A)	ATOM 1	ATOM 2	DISTANCE BETWEEN (°A)
65 Oδ1	157 Nδ1	3.9	65 Oδ1	157 Cε1	4.4
65 Oδ1	157 Cy	4.7	65 Oδ2	157 Nδ1	4.2
65 Oδ2	157 Cε1	4.5	132 N	336 O	4.2
132 N	161 Sy	4.3	132 Cα	336 O	3.2
132 Cα	161 Sy	4.8	132 CB	161 Sy	4.2
			132 CB	165 N	4.9
132 CB	336 O	3.8	132 Oy	161 Sy	3.6
132 C	336 O	3.6	132 C	134 N	4.1
			132 O	134 N	4.0
132 O	157 O	4.4			
132 O	336 O	4.8	134 N	157 O	2.8
134 N	157 C	4.0	134 N	157 Cδ2	4.4
134 N	157 N	4.5	134 N	157 Ne2	4.6
134 N	157 Cα	4.9	134 Cα	157 O	3.7
134 Cα	157 Cδ2	4.5	134 Cα	157 Ne2	4.5
134 Cα	157 N	4.5	134 Cα	157 C	4.8
134 CB	157 Ne2	3.1	134 CB	157 Cδ2	3.5
134 CB	157 Cε1	3.6	134 CB	157 O	3.9
134 CB	157 Cy	4.1	134 CB	157 Nδ1	4.2
134 CB	157 N	4.5	134 CB	157 C	4.7
134 Oy	157 Ne2	2.6	134 Oy	157 Cδ2	2.7

Fig. 18C

ATOM 1	ATOM 2	DISTANCE BETWEEN (°A)	ATOM 1	ATOM 2	DISTANCE BETWEEN (°A)
134 Oy	157 Cε1	2.8	134 Oy	157 Cy	3.0
134 Oy	157 Nδ1	3.0	134 Oy	157 N	3.3
134 Oy	157 O	3.3	134 Oy	157 C	3.8
134 Oy	157 Cα	3.9	134 Oy	157 Cβ	3.9
134 C	157 O	3.9	134 C	157 N	4.0
134 C	157 C	4.9	134 O	157 N	2.9
134 O	157 O	3.3	134 O	157 Cα	4.1
134 O	157 C	4.2	134 O	157 Cy	4.8
134 O	157 Cδ2	4.8			
165 Cα	166 N	2.4	165 Cα	166 Cα	3.8
165 Cα	166 O	4.1	165 Cα	166 C	4.3
165 Cα	166 Cβ	4.8	165 Cβ	166 N	3.1
165 Cβ	166 Cα	4.5	165 C	166 N	1.3
165 C	166 Cα	2.4	165 C	166 C	3.0
165 C	166 O	3.2	165 C	166 Cβ	3.7
165 C	166 Cy	4.4	165 O	166 N	2.3
165 O	166 Cα	2.8	165 O	166 C	3.1
165 O	166 O	3.5	165 O	166 Cβ	4.2
165 O	166 Cy	4.9	166 Cβ	336 O	4.8
166 Cδ	336 O	4.5	166 Nε	336 O	3.2
166 CZ	336 O	3.3	166 NH1	336 O	2.7
166 NH2	336 O	4.7			

Fig. 19A

<u>ATOM 1</u>	<u>MIDDLE ATOM</u>	<u>ATOM 3</u>	<u>ANGLE °</u>
63Ce1	63Nd1	157Ne2	134
63Cy	63Nd1	157Ne2	118
63Ne2	63Nd1	157Ne2	168
63Cd2	63Nd1	157Ne2	155
63Cb	63Nd1	157Ne2	80
63Ca	63Nd1	157Ne2	70
63Nd1	63Ce1	132Oy	146
63Nd1	63Ce1	132Cb	147
63Ne2	63Ce1	132Oy	89
63Ne2	63Ce1	132Cb	93
63Cd2	63Ce1	132Oy	123
63Cd2	63Ce1	132Cb	127
63Cy	63Ce1	132Oy	149
63Cy	63Ce1	132Cb	154
132Oy	63Ce1	132Cb	5
63Cb	63Ce1	132Cb	158
63Ce1	63Ne2	132Oy	67
63Cd2	63Ne2	132Oy	153
63Nd1	63Ne2	132Oy	98
63Cy	63Ne2	132Oy	130

Fig. 19B

<u>ATOM 1</u>	<u>MIDDLE ATOM</u>	<u>ATOM 3</u>	<u>ANGLE °</u>
63CB	63Ne2	132Oy	136
63Ca	63C	65N	153
63CB	63C	65N	152
63N	63C	65N	146
63C	63O	65N	103
63C	63O	65Ca	108
63Ca	63O	65N	130
63Ca	63O	65Ca	128
63CB	63O	65N	162
63CB	63O	65Ca	159
65N	63O	65Ca	18
63N	63O	65Ca	121
65Ca	65N	63O	125
65Ca	65N	63C	130
65CB	65N	63O	108
65CB	65N	63C	124
65C	65N	63O	152
65C	65N	63C	146
63O	65N	63C	20
65Cy	65N	63C	101
65N	65CA	63O	38

Fig. 19C

<u>ATOM 1</u>	<u>MIDDLE ATOM</u>	<u>ATOM 3</u>	<u>ANGLE °</u>
65C	65C α	63O	152
65CB	65C α	63O	96
65O	65C α	63O	164
65C γ	65C α	63O	83
65O δ 1	65C α	63O	86
65O δ 2	65C α	63O	76
65C γ	65O δ 1	157N δ 1	107
65O δ 2	65O δ 1	157N δ 1	83
65CB	65O δ 1	157N δ 1	131
65C α	65O δ 1	157N δ 1	129
65O	65O δ 1	157N δ 1	160
65C	65O δ 1	157N δ 1	146
65N	65O δ 1	157N δ 1	110
132O γ	132CB	63C ϵ 1	11
132C α	132CB	63C ϵ 1	111
132N	132CB	63C ϵ 1	112
132C	132CB	63C ϵ 1	83
132O	132CB	63C ϵ 1	71
132CB	132O γ	63C ϵ 1	164
132CB	132O γ	63N ϵ 2	163
132C α	132O γ	63C ϵ 1	139

Fig. 19D

<u>ATOM 1</u>	<u>MIDDLE ATOM</u>	<u>ATOM 3</u>	<u>ANGLE °</u>
132C α	132O γ	63N ϵ 2	162
132C	132O γ	63C ϵ 1	109
132C	132O γ	63N ϵ 2	133
63C ϵ 1	132O γ	63N ϵ 2	24
132N	132O γ	63N ϵ 2	148
157C γ	157N δ 1	65O δ 1	119
157N ϵ 2	157N δ 1	65O δ 1	125
157C δ 2	157N δ 1	65O δ 1	131
157C β	157N δ 1	65O δ 1	102
157C α	157N δ 1	65O δ 1	121
157N	157N δ 1	65O δ 1	130
157C ϵ 1	157N ϵ 2	63N δ 1	128
157C δ 2	157N ϵ 2	63N δ 1	126
157N δ 1	157N ϵ 2	63N δ 1	161
157C γ	157N ϵ 2	63N δ 1	160

Fig. 20

	Phi $C_n-1-N_n-C_n-C$	Psi $N-CA-C-N_{n+1}$	Omega 1 $CA_n-1-C_n-1-N_n-CA_n$	Omega 2 $CA_n-C_n-N_{n+1}-CA_{n+1}$	Chi1 $N-CA-CB-CG$	Chi2 $CA-CD-CG-XD$
Ser132	-152	133	176	-176	86	-
His63	68	-4	-180	179	-47	-71
His157	177	180	-178	177	64	-123
Asp65	-66	-7	-178	177	-102	-33

Fig. 21A

CRYST1	58.7	58.7	131.0	90.00	90.00	90.00	P4322
SCALE1	0.01703	0.00000	0.00000			0.00000	
SCALE2	0.00000	0.01703	0.00000			0.00000	
SCALE3	0.00000	0.00000	0.00763			0.00000	
ATOM	1	CB	GLU	9	41.534	21.636	33.140 1.00 62.86
ATOM	4	N	GLU	9	42.716	22.008	30.930 1.00 62.91
ATOM	5	CA	GLU	9	41.969	21.019	31.798 1.00 63.33
ATOM	2	C	GLU	9	40.771	20.456	31.058 1.00 61.56
ATOM	3	O	GLU	9	40.829	19.324	30.627 1.00 62.88
ATOM	1	CB	GLU	9	41.534	21.636	33.140 1.00 62.86
ATOM	6	N	ALA	10	39.681	21.220	30.958 1.00 61.86
ATOM	7	CA	ALA	10	38.494	20.780	30.215 1.00 60.47
ATOM	9	C	ALA	10	38.939	20.765	28.752 1.00 60.20
ATOM	10	O	ALA	10	38.451	20.001	27.919 1.00 57.60
ATOM	8	CB	ALA	10	37.360	21.760	30.419 1.00 61.05
ATOM	11	N	VAL	11	39.861	21.668	28.448 1.00 60.59
ATOM	12	CA	VAL	11	40.454	21.740	27.121 1.00 61.51
ATOM	16	C	VAL	11	41.763	20.883	27.198 1.00 61.40
ATOM	17	O	VAL	11	42.895	21.400	27.320 1.00 65.52
ATOM	13	CB	VAL	11	40.674	23.242	26.691 1.00 62.09
ATOM	14	CG1	VAL	11	41.642	23.342	25.496 1.00 61.02
ATOM	15	CG2	VAL	11	39.311	23.891	26.339 1.00 53.35
ATOM	18	N	ALA	12	41.556	19.570	27.275 1.00 54.83
ATOM	19	CA	ALA	12	42.612	18.580	27.366 1.00 49.08
ATOM	21	C	ALA	12	42.120	17.568	26.386 1.00 45.83
ATOM	22	O	ALA	12	40.960	17.604	26.052 1.00 50.77
ATOM	20	CB	ALA	12	42.626	17.994	28.738 1.00 50.51
ATOM	23	N	PRO	13	42.934	16.581	25.996 1.00 42.62
ATOM	25	CA	PRO	13	42.385	15.631	25.020 1.00 38.99
ATOM	28	C	PRO	13	41.130	14.905	25.460 1.00 32.92
ATOM	29	O	PRO	13	40.847	14.770	26.649 1.00 35.39
ATOM	26	CB	PRO	13	43.542	14.642	24.782 1.00 41.06
ATOM	27	CG	PRO	13	44.740	15.396	25.178 1.00 43.00
ATOM	24	CD	PRO	13	44.266	16.145	26.423 1.00 44.44
ATOM	30	N	VAL	14	40.350	14.519	24.473 1.00 25.41
ATOM	31	CA	VAL	14	39.142	13.783	24.696 1.00 25.42
ATOM	35	C	VAL	14	39.339	12.569	23.782 1.00 26.70
ATOM	36	O	VAL	14	39.695	12.730	22.621 1.00 28.81
ATOM	32	CB	VAL	14	37.894	14.577	24.212 1.00 24.85
ATOM	33	CG1	VAL	14	36.626	13.806	24.489 1.00 27.96
ATOM	34	CG2	VAL	14	37.830	15.921	24.846 1.00 23.28
ATOM	37	N	TYR	15	39.277	11.368	24.335 1.00 22.49
ATOM	38	CA	TYR	15	39.378	10.173	23.541 1.00 18.63
ATOM	47	C	TYR	15	37.954	9.771	23.256 1.00 18.44
ATOM	48	O	TYR	15	37.058	10.063	24.033 1.00 20.57
ATOM	39	CB	TYR	15	40.080	9.085	24.306 1.00 21.59
ATOM	40	CG	TYR	15	41.542	9.405	24.478 1.00 27.13
ATOM	41	CD1	TYR	15	41.963	10.367	25.402 1.00 26.70

Fig. 21B

ATOM	43	CD2	TYR	15	42.515	8.744	23.703	1.00	29.84
ATOM	42	CE1	TYR	15	43.298	10.666	25.553	1.00	26.64
ATOM	44	CE2	TYR	15	43.843	9.027	23.845	1.00	28.52
ATOM	45	CZ	TYR	15	44.227	9.990	24.771	1.00	34.44
ATOM	46	OH	TYR	15	45.567	10.264	24.905	1.00	46.06
ATOM	49	N	VAL	16	37.732	9.203	22.080	1.00	20.53
ATOM	50	CA	VAL	16	36.414	8.756	21.649	1.00	17.84
ATOM	54	C	VAL	16	36.641	7.332	21.202	1.00	18.98
ATOM	55	O	VAL	16	37.738	7.005	20.763	1.00	20.12
ATOM	51	CB	VAL	16	35.810	9.664	20.532	1.00	15.49
ATOM	52	CG1	VAL	16	36.785	9.863	19.365	1.00	12.77
ATOM	53	CG2	VAL	16	34.516	9.079	20.057	1.00	14.93
ATOM	56	N	GLY	17	35.666	6.447	21.398	1.00	19.44
ATOM	57	CA	GLY	17	35.897	5.069	21.006	1.00	14.35
ATOM	58	C	GLY	17	34.610	4.512	20.533	1.00	16.22
ATOM	59	O	GLY	17	33.562	5.031	20.868	1.00	18.87
ATOM	60	N	GLY	18	34.669	3.500	19.693	1.00	18.00
ATOM	61	CA	GLY	18	33.436	2.941	19.230	1.00	16.95
ATOM	62	C	GLY	18	33.640	2.066	18.039	1.00	19.29
ATOM	63	O	GLY	18	34.723	1.998	17.490	1.00	20.24
ATOM	64	N	PHE	19	32.564	1.417	17.636	1.00	22.41
ATOM	65	CA	PHE	19	32.586	0.545	16.504	1.00	27.48
ATOM	73	C	PHE	19	32.296	1.338	15.238	1.00	29.03
ATOM	74	O	PHE	19	31.310	2.084	15.168	1.00	28.29
ATOM	66	CB	PHE	19	31.546	-0.587	16.696	1.00	32.20
ATOM	67	CG	PHE	19	31.959	-1.632	17.741	1.00	38.36
ATOM	68	CD1	PHE	19	31.758	-1.398	19.105	1.00	35.34
ATOM	69	CD2	PHE	19	32.627	-2.812	17.356	1.00	36.45
ATOM	70	CE1	PHE	19	32.219	-2.302	20.041	1.00	34.55
ATOM	71	CE2	PHE	19	33.093	-3.731	18.297	1.00	33.01
ATOM	72	CZ	PHE	19	32.895	-3.479	19.631	1.00	37.50
ATOM	75	N	LEU	20	33.196	1.196	14.266	1.00	30.89
ATOM	76	CA	LEU	20	33.072	1.812	12.942	1.00	32.67
ATOM	81	C	LEU	20	32.215	0.912	12.037	1.00	34.96
ATOM	82	O	LEU	20	31.651	1.377	11.031	1.00	31.94
ATOM	77	CB	LEU	20	34.435	1.915	12.279	1.00	33.81
ATOM	78	CG	LEU	20	35.361	2.921	12.913	1.00	34.20
ATOM	79	CD1	LEU	20	36.708	2.830	12.254	1.00	36.26
ATOM	80	CD2	LEU	20	34.756	4.270	12.701	1.00	34.94
ATOM	83	N	ALA	21	32.146	-0.374	12.400	1.00	35.25
ATOM	84	CA	ALA	21	31.410	-1.366	11.627	1.00	35.19
ATOM	86	C	ALA	21	31.222	-2.658	12.385	1.00	35.36
ATOM	87	O	ALA	21	32.124	-3.155	13.038	1.00	35.57
ATOM	85	CB	ALA	21	32.166	-1.667	10.323	1.00	36.73
ATOM	88	N	ARG	22	30.051	-3.230	12.240	1.00	37.54
ATOM	89	CA	ARG	22	29.744	-4.481	12.881	1.00	42.49
ATOM	97	C	ARG	22	29.800	-5.638	11.909	1.00	43.79
ATOM	98	O	ARG	22	29.916	-5.466	10.705	1.00	47.98
ATOM	90	CB	ARG	22	28.338	-4.417	13.461	1.00	46.25
ATOM	91	CG	ARG	22	28.258	-3.651	14.759	1.00	49.18
ATOM	92	CD	ARG	22	28.025	-4.622	15.889	1.00	50.35
ATOM	93	NE	ARG	22	28.767	-4.220	17.069	1.00	47.50
ATOM	94	CZ	ARG	22	28.661	-4.817	18.243	1.00	43.85
ATOM	95	NH1	ARG	22	27.852	-5.850	18.385	1.00	43.35

Fig. 21C

ATOM	96	NH2	ARG	22	29.377	-4.381	19.267	1.00	48.14
ATOM	99	N	TYR	23	29.841	-6.824	12.480	1.00	45.08
ATOM	100	CA	TYR	23	29.810	-8.085	11.765	1.00	43.13
ATOM	109	C	TYR	23	28.553	-8.677	12.448	1.00	51.17
ATOM	110	O	TYR	23	28.269	-9.862	12.384	1.00	51.37
ATOM	101	CB	TYR	23	31.083	-8.871	12.084	1.00	33.90
ATOM	102	CG	TYR	23	32.396	-8.126	11.774	1.00	28.23
ATOM	103	CD1	TYR	23	32.413	-6.989	11.001	1.00	28.88
ATOM	105	CD2	TYR	23	33.617	-8.560	12.284	1.00	31.62
ATOM	104	CE1	TYR	23	33.609	-6.297	10.744	1.00	28.45
ATOM	106	CE2	TYR	23	34.828	-7.870	12.033	1.00	26.20
ATOM	107	CZ	TYR	23	34.808	-6.738	11.272	1.00	26.64
ATOM	108	OH	TYR	23	35.955	-5.981	11.093	1.00	29.32
ATOM	111	N	ASP	24	27.851	-7.762	13.130	1.00	58.25
ATOM	112	CA	ASP	24	26.614	-7.886	13.918	1.00	63.11
ATOM	117	C	ASP	24	26.435	-8.359	15.386	1.00	63.57
ATOM	118	O	ASP	24	25.267	-8.531	15.810	1.00	63.99
ATOM	113	CB	ASP	24	25.442	-8.280	13.038	1.00	61.93
ATOM	114	CG	ASP	24	24.707	-7.048	12.545	1.00	64.79
ATOM	115	OD1	ASP	24	24.278	-6.214	13.412	1.00	65.40
ATOM	116	OD2	ASP	24	24.642	-6.866	11.307	1.00	63.98
ATOM	123	N	ALA	56	47.806	7.903	12.460	1.00	59.91
ATOM	124	CA	ALA	56	46.875	7.183	11.545	1.00	58.34
ATOM	121	C	ALA	56	45.851	8.180	11.008	1.00	55.13
ATOM	122	O	ALA	56	46.087	9.389	11.060	1.00	55.11
ATOM	120	CB	ALA	56	46.172	6.018	12.291	1.00	58.09
ATOM	125	N	LEU	57	44.745	7.649	10.483	1.00	51.20
ATOM	126	CA	LEU	57	43.641	8.405	9.919	1.00	43.58
ATOM	131	C	LEU	57	43.284	9.682	10.678	1.00	44.00
ATOM	132	O	LEU	57	43.308	9.706	11.912	1.00	39.30
ATOM	127	CB	LEU	57	42.409	7.514	9.863	1.00	41.84
ATOM	128	CG	LEU	57	42.544	6.214	9.086	1.00	38.95
ATOM	129	CD1	LEU	57	41.181	5.670	8.644	1.00	36.90
ATOM	130	CD2	LEU	57	43.363	6.560	7.902	1.00	35.63
ATOM	133	N	PRO	58	43.002	10.778	9.940	1.00	43.35
ATOM	135	CA	PRO	58	42.646	12.015	10.617	1.00	40.99
ATOM	138	C	PRO	58	41.187	11.849	11.033	1.00	39.53
ATOM	139	O	PRO	58	40.395	11.143	10.392	1.00	37.00
ATOM	136	CB	PRO	58	42.808	13.062	9.516	1.00	40.54
ATOM	137	CG	PRO	58	42.298	12.347	8.350	1.00	39.45
ATOM	134	CD	PRO	58	42.912	10.958	8.477	1.00	42.41
ATOM	140	N	LEU	59	40.884	12.419	12.181	1.00	37.87
ATOM	141	CA	LEU	59	39.565	12.373	12.748	1.00	34.28
ATOM	146	C	LEU	59	39.054	13.731	12.336	1.00	30.93
ATOM	147	O	LEU	59	39.756	14.741	12.489	1.00	34.98
ATOM	142	CB	LEU	59	39.670	12.338	14.293	1.00	32.87
ATOM	143	CG	LEU	59	39.170	11.239	15.237	1.00	28.44
ATOM	144	CD1	LEU	59	39.064	11.797	16.680	1.00	28.76
ATOM	145	CD2	LEU	59	37.828	10.763	14.787	1.00	26.44
ATOM	148	N	ASN	60	37.887	13.774	11.740	1.00	29.17
ATOM	149	CA	ASN	60	37.328	15.059	11.422	1.00	31.43
ATOM	154	C	ASN	60	35.868	15.099	11.806	1.00	29.73
ATOM	155	O	ASN	60	35.281	14.081	12.205	1.00	30.65
ATOM	150	CB	ASN	60	37.535	15.437	9.959	1.00	31.90

Fig. 21D

ATOM	151	CG	ASN	60	36.819	14.540	9.016	1.00	28.44
ATOM	152	OD1	ASN	60	35.633	14.283	9.153	1.00	31.36
ATOM	153	ND2	ASN	60	37.534	14.091	8.003	1.00	35.05
ATOM	156	N	ILE	61	35.295	16.281	11.678	1.00	26.50
ATOM	157	CA	ILE	61	33.908	16.483	12.017	1.00	31.39
ATOM	162	C	ILE	61	33.008	16.414	10.755	1.00	32.16
ATOM	163	O	ILE	61	33.238	17.096	9.772	1.00	34.15
ATOM	158	CB	ILE	61	33.695	17.843	12.810	1.00	27.75
ATOM	160	CG1	ILE	61	34.467	17.856	14.134	1.00	17.65
ATOM	159	CG2	ILE	61	32.244	18.075	13.075	1.00	25.73
ATOM	161	CD1	ILE	61	34.057	16.786	15.063	1.00	19.49
ATOM	164	N	ASN	62	32.068	15.482	10.778	1.00	34.30
ATOM	165	CA	ASN	62	31.110	15.305	9.727	1.00	36.14
ATOM	170	C	ASN	62	31.724	15.247	8.327	1.00	38.20
ATOM	171	O	ASN	62	31.133	15.735	7.353	1.00	40.25
ATOM	166	CB	ASN	62	30.084	16.424	9.855	1.00	41.53
ATOM	167	CG	ASN	62	28.668	15.915	9.839	1.00	50.38
ATOM	168	OD1	ASN	62	27.901	16.093	10.807	1.00	53.37
ATOM	169	ND2	ASN	62	28.295	15.283	8.734	1.00	52.09
ATOM	172	N	HIS	63	32.904	14.647	8.212	1.00	37.80
ATOM	173	CA	HIS	63	33.585	14.536	6.920	1.00	38.53
ATOM	174	C	HIS	63	34.089	15.835	6.297	1.00	40.67
ATOM	175	O	HIS	63	34.665	15.795	5.217	1.00	46.88
ATOM	176	CB	HIS	63	32.692	13.894	5.883	1.00	33.48
ATOM	177	CG	HIS	63	32.012	12.655	6.360	1.00	34.46
ATOM	178	ND1	HIS	63	32.650	11.463	6.594	1.00	32.89
ATOM	179	CD2	HIS	63	30.684	12.410	6.543	1.00	33.18
ATOM	181	CE1	HIS	63	31.716	10.546	6.885	1.00	32.87
ATOM	180	NE2	HIS	63	30.502	11.073	6.870	1.00	35.51
ATOM	182	N	ASP	64	33.824	16.981	6.904	1.00	38.28
ATOM	183	CA	ASP	64	34.302	18.233	6.359	1.00	36.79
ATOM	188	C	ASP	64	35.792	18.139	6.510	1.00	40.50
ATOM	189	O	ASP	64	36.266	18.264	7.625	1.00	41.47
ATOM	184	CB	ASP	64	33.819	19.371	7.229	1.00	39.15
ATOM	185	CG	ASP	64	34.280	20.729	6.740	1.00	45.12
ATOM	186	OD1	ASP	64	35.289	20.832	5.997	1.00	47.63
ATOM	187	OD2	ASP	64	33.616	21.727	7.130	1.00	52.05
ATOM	190	N	ASP	65	36.539	18.046	5.407	1.00	42.46
ATOM	191	CA	ASP	65	37.992	17.914	5.497	1.00	43.12
ATOM	196	C	ASP	65	38.781	19.063	6.051	1.00	42.62
ATOM	197	O	ASP	65	39.992	18.935	6.265	1.00	43.71
ATOM	192	CB	ASP	65	38.616	17.402	4.209	1.00	46.43
ATOM	193	CG	ASP	65	38.980	15.918	4.294	1.00	58.98
ATOM	194	OD1	ASP	65	39.355	15.409	5.390	1.00	62.06
ATOM	195	OD2	ASP	65	38.867	15.231	3.256	1.00	67.86
ATOM	198	N	THR	66	38.112	20.183	6.303	1.00	41.56
ATOM	199	CA	THR	66	38.793	21.333	6.900	1.00	40.94
ATOM	203	C	THR	66	38.621	21.342	8.441	1.00	39.77
ATOM	204	O	THR	66	39.348	22.049	9.154	1.00	41.93
ATOM	200	CB	THR	66	38.283	22.658	6.289	1.00	43.33
ATOM	201	OG1	THR	66	37.049	23.050	6.909	1.00	47.53
ATOM	202	CG2	THR	66	38.039	22.477	4.801	1.00	39.24
ATOM	205	N	ALA	67	37.673	20.522	8.925	1.00	34.31
ATOM	206	CA	ALA	67	37.306	20.377	10.332	1.00	25.72

Fig. 21E

ATOM	208	C	ALA	67	38.006	19.185	10.954	1.00	27.24
ATOM	209	O	ALA	67	37.352	18.359	11.559	1.00	28.36
ATOM	207	CB	ALA	67	35.819	20.168	10.426	1.00	18.91
ATOM	210	N	VAL	68	39.312	19.045	10.772	1.00	27.63
ATOM	211	CA	VAL	68	40.008	17.902	11.341	1.00	27.26
ATOM	215	C	VAL	68	40.308	18.224	12.773	1.00	28.89
ATOM	216	O	VAL	68	40.919	19.237	13.076	1.00	28.74
ATOM	212	CB	VAL	68	41.239	17.566	10.550	1.00	26.97
ATOM	213	CG1	VAL	68	42.171	16.655	11.343	1.00	23.43
ATOM	214	CG2	VAL	68	40.778	16.883	9.269	1.00	22.68
ATOM	217	N	VAL	69	39.863	17.351	13.665	1.00	29.30
ATOM	218	CA	VAL	69	39.999	17.623	15.083	1.00	27.08
ATOM	222	C	VAL	69	40.970	16.778	15.843	1.00	27.21
ATOM	223	O	VAL	69	41.182	17.025	17.020	1.00	27.27
ATOM	219	CB	VAL	69	38.637	17.547	15.765	1.00	26.23
ATOM	220	CG1	VAL	69	37.617	18.423	14.998	1.00	24.62
ATOM	221	CG2	VAL	69	38.168	16.117	15.812	1.00	24.71
ATOM	224	N	GLY	70	41.574	15.813	15.160	1.00	25.43
ATOM	225	CA	GLY	70	42.537	14.934	15.784	1.00	26.47
ATOM	226	C	GLY	70	42.859	13.756	14.883	1.00	29.60
ATOM	227	O	GLY	70	42.546	13.779	13.694	1.00	32.40
ATOM	228	N	HIS	71	43.355	12.677	15.475	1.00	29.41
ATOM	229	CA	HIS	71	43.770	11.490	14.740	1.00	28.39
ATOM	236	C	HIS	71	43.259	10.230	15.432	1.00	29.26
ATOM	237	O	HIS	71	42.832	10.275	16.566	1.00	32.50
ATOM	230	CB	HIS	71	45.280	11.442	14.786	1.00	31.71
ATOM	231	CG	HIS	71	45.818	11.420	16.188	1.00	36.79
ATOM	233	ND1	HIS	71	45.936	12.563	16.953	1.00	39.46
ATOM	232	CD2	HIS	71	46.206	10.396	16.979	1.00	40.16
ATOM	234	CE1	HIS	71	46.378	12.240	18.155	1.00	45.55
ATOM	235	NE2	HIS	71	46.550	10.931	18.201	1.00	44.70
ATOM	238	N	VAL	72	43.368	9.097	14.762	1.00	30.12
ATOM	239	CA	VAL	72	42.964	7.819	15.302	1.00	27.63
ATOM	243	C	VAL	72	44.211	7.228	15.906	1.00	31.61
ATOM	244	O	VAL	72	45.226	7.100	15.218	1.00	35.21
ATOM	240	CB	VAL	72	42.524	6.905	14.206	1.00	25.86
ATOM	241	CG1	VAL	72	42.140	5.564	14.755	1.00	26.21
ATOM	242	CG2	VAL	72	41.387	7.541	13.450	1.00	28.96
ATOM	245	N	ALA	73	44.134	6.908	17.199	1.00	31.08
ATOM	246	CA	ALA	73	45.236	6.329	17.966	1.00	31.72
ATOM	248	C	ALA	73	45.424	4.802	17.790	1.00	31.44
ATOM	249	O	ALA	73	46.555	4.322	17.828	1.00	35.11
ATOM	247	CB	ALA	73	45.061	6.657	19.451	1.00	23.78
ATOM	250	N	ALA	74	44.325	4.069	17.600	1.00	28.56
ATOM	251	CA	ALA	74	44.327	2.621	17.467	1.00	25.12
ATOM	253	C	ALA	74	43.077	2.149	16.749	1.00	27.57
ATOM	254	O	ALA	74	42.078	2.844	16.705	1.00	33.33
ATOM	252	CB	ALA	74	44.359	2.009	18.806	1.00	22.03
ATOM	255	N	MET	75	43.137	0.955	16.195	1.00	27.43
ATOM	256	CA	MET	75	42.032	0.350	15.465	1.00	30.16
ATOM	261	C	MET	75	42.200	-1.132	15.734	1.00	31.88
ATOM	262	O	MET	75	43.309	-1.564	16.048	1.00	38.15
ATOM	257	CB	MET	75	42.137	0.620	13.972	1.00	31.38
ATOM	258	CG	MET	75	41.463	1.885	13.478	1.00	34.40

Fig. 21F

ATOM	259	SD	MET	75	40.518	-1.487	11.975	1.00	44.35
ATOM	260	CE	MET	75	40.613	2.988	11.127	1.00	45.26
ATOM	263	N	GLN	76	41.134	-1.911	15.647	1.00	30.46
ATOM	264	CA	GLN	76	41.232	-3.320	15.949	1.00	33.80
ATOM	270	C	GLN	76	40.013	-4.010	15.501	1.00	36.87
ATOM	271	O	GLN	76	38.928	-3.575	15.871	1.00	36.72
ATOM	265	CB	GLN	76	41.247	-3.535	17.461	1.00	35.06
ATOM	266	CG	GLN	76	42.572	-3.388	18.123	1.00	38.58
ATOM	267	CD	GLN	76	43.245	-4.710	18.319	1.00	44.71
ATOM	268	OE1	GLN	76	42.645	-5.648	18.850	1.00	47.69
ATOM	269	NE2	GLN	76	44.494	-4.815	17.870	1.00	49.16
ATOM	272	N	SER	77	40.158	-5.100	14.747	1.00	42.23
ATOM	273	CA	SER	77	38.970	-5.873	14.356	1.00	46.68
ATOM	276	C	SER	77	38.752	-6.793	15.532	1.00	48.65
ATOM	277	O	SER	77	39.582	-7.622	15.876	1.00	53.74
ATOM	274	CB	SER	77	39.144	-6.714	13.070	1.00	50.01
ATOM	275	OG	SER	77	37.898	-7.259	12.608	1.00	45.65
ATOM	278	N	VAL	78	37.747	-6.446	16.284	1.00	50.11
ATOM	279	CA	VAL	78	37.348	-7.206	17.421	1.00	49.45
ATOM	283	C	VAL	78	36.405	-8.256	16.781	1.00	51.72
ATOM	284	O	VAL	78	35.999	-8.122	15.618	1.00	54.42
ATOM	280	CB	VAL	78	36.661	-6.225	18.365	1.00	49.01
ATOM	281	CG1	VAL	78	35.336	-6.760	18.923	1.00	49.51
ATOM	282	CG2	VAL	78	37.647	-5.805	19.403	1.00	48.72
ATOM	285	N	ARG	79	36.070	-9.305	17.508	1.00	49.34
ATOM	286	CA	ARG	79	35.206	-10.325	16.948	1.00	50.82
ATOM	289	C	ARG	79	33.859	-9.834	16.411	1.00	48.32
ATOM	290	O	ARG	79	33.346	-10.394	15.419	1.00	48.68
ATOM	287	CB	ARG	79	34.988	-11.436	17.970	1.00	55.34
ATOM	288	CG	ARG	79	34.603	-10.892	19.226	1.00	64.21
ATOM	291	N	ASP	80	33.285	-8.826	17.080	1.00	42.03
ATOM	292	CA	ASP	80	31.985	-8.266	16.700	1.00	35.98
ATOM	297	C	ASP	80	32.025	-7.108	15.713	1.00	33.25
ATOM	298	O	ASP	80	30.967	-6.626	15.287	1.00	28.18
ATOM	293	CB	ASP	80	31.267	-7.762	17.920	1.00	39.29
ATOM	294	CG	ASP	80	30.521	-8.820	18.618	1.00	44.58
ATOM	295	OD1	ASP	80	29.645	-9.409	17.977	1.00	44.97
ATOM	296	OD2	ASP	80	30.787	-9.041	19.825	1.00	53.61
ATOM	299	N	GLY	81	33.221	-6.611	15.411	1.00	28.25
ATOM	300	CA	GLY	81	33.323	-5.504	14.485	1.00	24.48
ATOM	301	C	GLY	81	34.685	-4.857	14.471	1.00	24.50
ATOM	302	O	GLY	81	35.671	-5.398	14.951	1.00	26.60
ATOM	303	N	LEU	82	34.767	-3.672	13.925	1.00	24.01
ATOM	304	CA	LEU	82	36.056	-3.040	13.885	1.00	28.02
ATOM	309	C	LEU	82	35.941	-1.861	14.785	1.00	30.82
ATOM	310	O	LEU	82	35.154	-0.944	14.555	1.00	35.51
ATOM	305	CB	LEU	82	36.409	-2.661	12.459	1.00	27.07
ATOM	306	CG	LEU	82	37.223	-1.417	12.186	1.00	24.56
ATOM	307	CD1	LEU	82	38.730	-1.657	12.349	1.00	19.11
ATOM	308	CD2	LEU	82	36.823	-1.057	10.741	1.00	21.38
ATOM	311	N	PHE	83	36.606	-2.006	15.911	1.00	32.41
ATOM	312	CA	PHE	83	36.640	-1.012	16.959	1.00	29.23
ATOM	320	C	PHE	83	37.720	0.060	16.697	1.00	30.66
ATOM	321	O	PHE	83	38.838	-0.251	16.328	1.00	34.10

Fig. 21G

ATOM	313	CB	PHE	83	36.869	-1.732	18.297	1.00	24.26
ATOM	314	CG	PHE	83	36.705	-0.861	19.459	1.00	19.69
ATOM	315	CD1	PHE	83	35.439	-0.645	19.996	1.00	24.66
ATOM	316	CD2	PHE	83	37.785	-0.193	19.983	1.00	17.19
ATOM	317	CE1	PHE	83	35.260	0.237	21.056	1.00	23.22
ATOM	318	CE2	PHE	83	37.626	0.684	21.027	1.00	21.02
ATOM	319	CZ	PHE	83	36.363	0.903	21.565	1.00	25.05
ATOM	322	N	CYS	84	37.397	1.316	16.949	1.00	31.52
ATOM	323	CA	CYS	84	38.326	2.398	16.725	1.00	32.29
ATOM	326	C	CYS	84	38.381	3.256	17.967	1.00	31.97
ATOM	327	O	CYS	84	37.351	3.485	18.598	1.00	34.84
ATOM	324	CB	CYS	84	37.804	3.230	15.542	1.00	37.31
ATOM	325	SG	CYS	84	38.364	4.960	15.396	1.00	40.75
ATOM	328	N	LEU	85	39.568	3.695	18.351	1.00	28.35
ATOM	329	CA	LEU	85	39.695	4.584	19.491	1.00	29.63
ATOM	334	C	LEU	85	40.407	5.763	18.897	1.00	31.03
ATOM	335	O	LEU	85	41.477	5.580	18.326	1.00	33.68
ATOM	330	CB	LEU	85	40.579	3.986	20.572	1.00	33.66
ATOM	331	CG	LEU	85	41.167	4.969	21.577	1.00	33.78
ATOM	332	CD1	LEU	85	40.107	5.579	22.470	1.00	39.41
ATOM	333	CD2	LEU	85	42.107	4.201	22.416	1.00	39.36
ATOM	336	N	GLY	86	39.794	6.944	18.978	1.00	28.95
ATOM	337	CA	GLY	86	40.367	8.166	18.435	1.00	24.27
ATOM	338	C	GLY	86	40.800	9.198	19.473	1.00	22.24
ATOM	339	O	GLY	86	40.508	9.093	20.657	1.00	21.56
ATOM	340	N	CYS	87	41.483	10.230	19.033	1.00	21.98
ATOM	341	CA	CYS	87	41.929	11.226	19.966	1.00	26.67
ATOM	344	C	CYS	87	41.635	12.611	19.412	1.00	31.30
ATOM	345	O	CYS	87	42.197	13.020	18.395	1.00	34.32
ATOM	342	CB	CYS	87	43.424	11.079	20.251	1.00	24.73
ATOM	343	SG	CYS	87	43.947	12.153	21.635	1.00	48.28
ATOM	346	N	VAL	88	40.719	13.320	20.065	1.00	34.34
ATOM	347	CA	VAL	88	40.372	14.665	19.672	1.00	32.23
ATOM	351	C	VAL	88	41.411	15.564	20.367	1.00	33.80
ATOM	352	O	VAL	88	41.443	15.643	21.585	1.00	35.25
ATOM	348	CB	VAL	88	38.938	14.996	20.090	1.00	28.12
ATOM	349	CG1	VAL	88	38.673	16.482	19.820	1.00	25.49
ATOM	350	CG2	VAL	88	37.943	14.080	19.324	1.00	16.62
ATOM	353	N	THR	89	42.318	16.149	19.584	1.00	33.79
ATOM	354	CA	THR	89	43.390	16.972	20.124	1.00	33.14
ATOM	358	C	THR	89	43.458	18.424	19.711	1.00	32.49
ATOM	359	O	THR	89	44.239	19.152	20.289	1.00	33.05
ATOM	355	CB	THR	89	44.780	16.363	19.823	1.00	35.08
ATOM	356	OG1	THR	89	44.885	16.070	18.424	1.00	35.69
ATOM	357	CG2	THR	89	45.009	15.072	20.648	1.00	36.62
ATOM	360	N	SER	90	42.649	18.857	18.742	1.00	31.80
ATOM	361	CA	SER	90	42.674	20.239	18.276	1.00	27.06
ATOM	364	C	SER	90	42.263	21.289	19.312	1.00	28.01
ATOM	365	O	SER	90	41.084	21.405	19.640	1.00	30.53
ATOM	362	CB	SER	90	41.769	20.375	17.083	1.00	24.45
ATOM	363	OG	SER	90	41.487	21.744	16.873	1.00	22.16
ATOM	366	N	PRO	91	43.200	22.154	19.748	1.00	30.63
ATOM	368	CA	PRO	91	42.806	23.158	20.748	1.00	29.38
ATOM	371	C	PRO	91	41.789	24.184	20.273	1.00	30.13

Fig. 21H

ATOM	372	O	PRO	91	41.055	24.746	21.112	1.00	31.90
ATOM	369	CB	PRO	91	44.136	23.790	21.161	1.00	28.63
ATOM	370	CG	PRO	91	45.019	23.604	19.960	1.00	27.74
ATOM	367	CD	PRO	91	44.647	22.232	19.450	1.00	30.89
ATOM	373	N	ARG	92	41.746	24.426	18.948	1.00	29.72
ATOM	374	CA	ARG	92	40.793	25.388	18.357	1.00	30.28
ATOM	382	C	ARG	92	39.422	24.813	18.474	1.00	26.46
ATOM	383	O	ARG	92	38.500	25.516	18.754	1.00	28.07
ATOM	375	CB	ARG	92	41.072	25.701	16.875	1.00	35.94
ATOM	376	CG	ARG	92	42.156	26.784	16.654	1.00	46.08
ATOM	377	CD	ARG	92	42.221	27.323	15.218	1.00	51.31
ATOM	378	NE	ARG	92	41.126	28.254	14.928	1.00	59.30
ATOM	379	CZ	ARG	92	40.071	27.975	14.151	1.00	63.79
ATOM	380	NH1	ARG	92	39.974	26.779	13.573	1.00	65.29
ATOM	381	NH2	ARG	92	39.106	28.885	13.941	1.00	60.53
ATOM	384	N	PHE	93	39.318	23.506	18.291	1.00	26.43
ATOM	385	CA	PHE	93	38.063	22.800	18.377	1.00	24.08
ATOM	393	C	PHE	93	37.615	22.748	19.812	1.00	26.54
ATOM	394	O	PHE	93	36.517	23.197	20.133	1.00	30.25
ATOM	386	CB	PHE	93	38.216	21.375	17.845	1.00	24.37
ATOM	387	CG	PHE	93	36.950	20.569	17.886	1.00	23.16
ATOM	388	CD1	PHE	93	35.801	21.031	17.290	1.00	18.00
ATOM	389	CD2	PHE	93	36.917	19.337	18.520	1.00	22.53
ATOM	390	CE1	PHE	93	34.646	20.274	17.327	1.00	21.51
ATOM	391	CE2	PHE	93	35.747	18.578	18.555	1.00	24.70
ATOM	392	CZ	PHE	93	34.618	19.047	17.955	1.00	20.70
ATOM	395	N	LEU	94	38.468	22.230	20.689	1.00	28.43
ATOM	396	CA	LEU	94	38.122	22.120	22.111	1.00	30.42
ATOM	401	C	LEU	94	37.648	23.446	22.718	1.00	31.64
ATOM	402	O	LEU	94	36.784	23.450	23.605	1.00	32.40
ATOM	397	CB	LEU	94	39.293	21.518	22.901	1.00	32.97
ATOM	398	CG	LEU	94	39.625	20.141	22.323	1.00	30.59
ATOM	399	CD1	LEU	94	40.883	19.552	22.918	1.00	28.68
ATOM	400	CD2	LEU	94	38.404	19.239	22.514	1.00	28.08
ATOM	403	N	GLU	95	38.148	24.568	22.186	1.00	31.10
ATOM	404	CA	GLU	95	37.751	25.887	22.666	1.00	29.37
ATOM	410	C	GLU	95	36.415	26.373	22.069	1.00	28.17
ATOM	411	O	GLU	95	35.689	27.175	22.674	1.00	30.64
ATOM	405	CB	GLU	95	38.882	26.890	22.431	1.00	31.01
ATOM	406	CG	GLU	95	38.583	28.321	22.898	1.00	35.53
ATOM	407	CD	GLU	95	38.293	28.450	24.401	1.00	39.93
ATOM	408	OE1	GLU	95	38.606	27.509	25.180	1.00	40.14
ATOM	409	OE2	GLU	95	37.756	29.521	24.805	1.00	41.17
ATOM	412	N	ILE	96	36.095	25.917	20.868	1.00	24.90
ATOM	413	CA	ILE	96	34.841	26.295	20.251	1.00	21.92
ATOM	418	C	ILE	96	33.860	25.605	21.175	1.00	22.41
ATOM	419	O	ILE	96	32.961	26.243	21.702	1.00	24.87
ATOM	414	CB	ILE	96	34.653	25.663	18.822	1.00	20.49
ATOM	416	CG1	ILE	96	35.710	26.127	17.819	1.00	17.09
ATOM	415	CG2	ILE	96	33.303	25.995	18.266	1.00	16.58
ATOM	417	CD1	ILE	96	35.603	27.514	17.437	1.00	16.51
ATOM	420	N	VAL	97	34.124	24.315	21.435	1.00	25.93
ATOM	421	CA	VAL	97	33.296	23.401	22.259	1.00	24.81
ATOM	425	C	VAL	97	33.099	23.764	23.722	1.00	24.82

Fig. 211

ATOM	426	O	VAL	97	32.004	23.616	24.258	1.00	24.18
ATOM	422	CB	VAL	97	33.814	21.934	22.180	1.00	22.94
ATOM	423	CG1	VAL	97	33.030	21.053	23.180	1.00	24.88
ATOM	424	CG2	VAL	97	33.629	21.408	20.770	1.00	11.21
ATOM	427	N	ARG	98	34.182	24.151	24.380	1.00	24.78
ATOM	428	CA	ARG	98	34.128	24.566	25.766	1.00	25.00
ATOM	436	C	ARG	98	33.222	25.783	25.945	1.00	24.90
ATOM	437	O	ARG	98	32.390	25.831	26.836	1.00	27.48
ATOM	429	CB	ARG	98	35.513	24.908	26.216	1.00	24.67
ATOM	430	CG	ARG	98	35.642	24.954	27.674	1.00	30.94
ATOM	431	CD	ARG	98	36.587	26.059	28.036	1.00	40.09
ATOM	432	NE	ARG	98	35.865	27.299	28.292	1.00	45.08
ATOM	433	CZ	ARG	98	36.326	28.500	27.970	1.00	46.47
ATOM	434	NH1	ARG	98	37.502	28.616	27.359	1.00	45.05
ATOM	435	NH2	ARG	98	35.600	29.576	28.247	1.00	46.19
ATOM	438	N	ARG	99	33.388	26.768	25.080	1.00	26.59
ATOM	439	CA	ARG	99	32.581	27.974	25.115	1.00	25.39
ATOM	447	C	ARG	99	31.137	27.637	24.814	1.00	26.34
ATOM	448	O	ARG	99	30.254	28.226	25.373	1.00	29.98
ATOM	440	CB	ARG	99	33.052	28.968	24.067	1.00	24.52
ATOM	441	CG	ARG	99	34.402	29.547	24.250	1.00	26.43
ATOM	442	CD	ARG	99	34.233	31.068	24.120	1.00	44.08
ATOM	443	NE	ARG	99	35.510	31.764	24.079	1.00	54.56
ATOM	444	CZ	ARG	99	36.330	31.766	23.024	1.00	63.35
ATOM	445	NH1	ARG	99	35.978	31.185	21.865	1.00	66.14
ATOM	446	NH2	ARG	99	37.495	32.405	23.101	1.00	65.49
ATOM	449	N	ALA	100	30.892	26.685	23.922	1.00	27.99
ATOM	450	CA	ALA	100	29.522	26.331	23.562	1.00	24.77
ATOM	452	C	ALA	100	28.801	25.587	24.662	1.00	25.30
ATOM	453	O	ALA	100	27.678	25.920	25.012	1.00	23.06
ATOM	451	CB	ALA	100	29.517	25.537	22.317	1.00	30.83
ATOM	454	N	SER	101	29.454	24.561	25.190	1.00	25.97
ATOM	455	CA	SER	101	28.929	23.745	26.290	1.00	26.37
ATOM	458	C	SER	101	28.422	24.590	27.453	1.00	26.29
ATOM	459	O	SER	101	27.470	24.217	28.123	1.00	26.57
ATOM	456	CB	SER	101	30.036	22.860	26.808	1.00	22.89
ATOM	457	OG	SER	101	31.081	23.690	27.274	1.00	33.20
ATOM	460	N	GLU	102	29.068	25.727	27.676	1.00	27.99
ATOM	461	CA	GLU	102	28.683	26.645	28.739	1.00	31.99
ATOM	467	C	GLU	102	27.291	27.253	28.565	1.00	33.82
ATOM	468	O	GLU	102	26.715	27.794	29.508	1.00	34.90
ATOM	462	CB	GLU	102	29.724	27.746	28.868	1.00	37.00
ATOM	463	CG	GLU	102	30.912	27.375	29.771	1.00	46.44
ATOM	464	CD	GLU	102	31.984	28.469	29.817	1.00	56.16
ATOM	465	OE1	GLU	102	31.632	29.690	29.843	1.00	59.34
ATOM	466	OE2	GLU	102	33.184	28.096	29.823	1.00	61.81
ATOM	469	N	LYS	103	26.747	27.161	27.357	1.00	34.52
ATOM	470	CA	LYS	103	25.415	27.670	27.063	1.00	29.61
ATOM	476	C	LYS	103	24.451	26.519	26.791	1.00	28.42
ATOM	477	O	LYS	103	23.349	26.726	26.298	1.00	31.71
ATOM	471	CB	LYS	103	25.477	28.566	25.834	1.00	32.12
ATOM	472	CG	LYS	103	26.549	29.591	25.948	1.00	34.88
ATOM	473	CD	LYS	103	26.152	30.615	26.953	1.00	35.23
ATOM	474	CE	LYS	103	24.836	31.229	26.511	1.00	41.33

Fig. 21J

ATOM	475	NZ	LYS	103	24.480	32.498	27.258	1.00	46.16
ATOM	478	N	SER	104	24.849	25.297	27.086	1.00	27.63
ATOM	479	CA	SER	104	23.959	24.201	26.824	1.00	28.05
ATOM	482	C	SER	104	23.211	23.788	28.069	1.00	33.45
ATOM	483	O	SER	104	23.812	23.562	29.120	1.00	37.03
ATOM	480	CB	SER	104	24.714	23.001	26.291	1.00	23.58
ATOM	481	OG	SER	104	23.791	21.958	26.049	1.00	19.53
ATOM	484	N	GLU	105	21.899	23.632	27.935	1.00	34.63
ATOM	485	CA	GLU	105	21.071	23.207	29.041	1.00	32.71
ATOM	491	C	GLU	105	21.307	21.744	29.247	1.00	31.79
ATOM	492	O	GLU	105	21.475	21.275	30.364	1.00	33.10
ATOM	486	CB	GLU	105	19.629	23.421	28.696	1.00	38.95
ATOM	487	CG	GLU	105	18.768	23.600	29.892	1.00	54.82
ATOM	488	CD	GLU	105	17.332	23.295	29.578	1.00	61.77
ATOM	489	OE1	GLU	105	16.845	23.846	28.549	1.00	64.22
ATOM	490	OE2	GLU	105	16.717	22.490	30.343	1.00	62.11
ATOM	493	N	LEU	106	21.371	21.011	28.149	1.00	29.89
ATOM	494	CA	LEU	106	21.597	19.586	28.261	1.00	29.47
ATOM	499	C	LEU	106	22.871	19.338	29.047	1.00	29.92
ATOM	500	O	LEU	106	22.864	18.576	29.995	1.00	32.83
ATOM	495	CB	LEU	106	21.700	18.940	26.881	1.00	29.36
ATOM	496	CG	LEU	106	22.014	17.438	26.834	1.00	30.11
ATOM	497	CD1	LEU	106	20.724	16.658	27.088	1.00	34.79
ATOM	498	CD2	LEU	106	22.655	17.040	25.487	1.00	28.82
ATOM	501	N	VAL	107	23.956	20.002	28.643	1.00	33.22
ATOM	502	CA	VAL	107	25.273	19.866	29.285	1.00	32.61
ATOM	506	C	VAL	107	25.260	20.293	30.764	1.00	35.86
ATOM	507	O	VAL	107	25.968	19.704	31.585	1.00	35.65
ATOM	503	CB	VAL	107	26.353	20.692	28.552	1.00	26.05
ATOM	504	CG1	VAL	107	27.542	20.895	29.465	1.00	20.60
ATOM	505	CG2	VAL	107	26.748	20.013	27.269	1.00	22.79
ATOM	508	N	SER	108	24.451	21.306	31.083	1.00	36.37
ATOM	509	CA	SER	108	24.336	21.808	32.439	1.00	37.26
ATOM	512	C	SER	108	23.612	20.862	33.377	1.00	35.98
ATOM	513	O	SER	108	23.861	20.897	34.555	1.00	38.67
ATOM	510	CB	SER	108	23.760	23.224	32.447	1.00	39.50
ATOM	511	OG	SER	108	24.648	24.081	31.701	1.00	49.13
ATOM	514	N	ARG	109	22.744	20.000	32.868	1.00	36.47
ATOM	515	CA	ARG	109	22.093	19.015	33.723	1.00	35.04
ATOM	523	C	ARG	109	23.129	17.948	34.150	1.00	35.68
ATOM	524	O	ARG	109	22.852	17.151	35.045	1.00	36.71
ATOM	516	CB	ARG	109	20.993	18.294	32.970	1.00	38.35
ATOM	517	CG	ARG	109	19.761	19.083	32.730	1.00	50.79
ATOM	518	CD	ARG	109	18.743	18.290	31.877	1.00	58.60
ATOM	519	NE	ARG	109	17.542	19.093	31.677	1.00	61.15
ATOM	520	CZ	ARG	109	16.771	19.512	32.683	1.00	64.92
ATOM	521	NH1	ARG	109	17.077	19.178	33.945	1.00	61.63
ATOM	522	NH2	ARG	109	15.719	20.303	32.444	1.00	66.50
ATOM	525	N	GLY	110	24.272	17.878	33.451	1.00	32.19
ATOM	526	CA	GLY	110	25.318	16.920	33.780	1.00	24.13
ATOM	527	C	GLY	110	24.970	15.456	33.563	1.00	26.01
ATOM	528	O	GLY	110	23.931	15.149	32.973	1.00	29.54
ATOM	529	N	PRO	111	25.827	14.524	34.036	1.00	24.15
ATOM	531	CA	PRO	111	25.726	13.077	33.956	1.00	24.37

Fig. 21K

ATOM	534	C	PRO	111	24.721	12.557	34.946	1.00	33.63
ATOM	535	O	PRO	111	24.270	13.302	35.813	1.00	34.08
ATOM	532	CB	PRO	111	27.102	12.620	34.398	1.00	21.65
ATOM	533	CG	PRO	111	27.936	13.798	34.342	1.00	24.20
ATOM	530	CD	PRO	111	27.045	14.868	34.761	1.00	22.63
ATOM	536	N	VAL	112	24.530	11.232	34.925	1.00	42.68
ATOM	537	CA	VAL	112	23.567	10.569	35.794	1.00	49.61
ATOM	541	C	VAL	112	23.782	10.487	37.266	1.00	51.99
ATOM	542	O	VAL	112	22.921	10.961	38.013	1.00	56.60
ATOM	538	CB	VAL	112	23.211	9.115	35.393	1.00	53.14
ATOM	539	CG1	VAL	112	22.457	9.090	34.072	1.00	56.14
ATOM	540	CG2	VAL	112	24.461	8.209	35.431	1.00	56.78
ATOM	543	N	SER	113	24.843	9.841	37.724	1.00	50.45
ATOM	544	CA	SER	113	24.890	9.737	39.161	1.00	56.14
ATOM	547	C	SER	113	26.187	9.891	39.864	1.00	56.87
ATOM	548	O	SER	113	26.360	10.882	40.575	1.00	62.69
ATOM	545	CB	SER	113	24.137	8.496	39.660	1.00	58.65
ATOM	546	OG	SER	113	22.966	8.848	40.388	1.00	63.80
ATOM	549	N	PRO	114	27.067	8.883	39.809	1.00	51.53
ATOM	551	CA	PRO	114	28.311	9.156	40.539	1.00	46.33
ATOM	554	C	PRO	114	29.374	9.770	39.640	1.00	42.61
ATOM	555	O	PRO	114	30.429	10.140	40.133	1.00	43.75
ATOM	552	CB	PRO	114	28.737	7.775	41.040	1.00	46.79
ATOM	553	CG	PRO	114	27.463	6.925	40.912	1.00	48.56
ATOM	550	CD	PRO	114	26.879	7.436	39.637	1.00	49.67
ATOM	556	N	LEU	115	29.087	9.854	38.332	1.00	39.27
ATOM	557	CA	LEU	115	30.011	10.410	37.327	1.00	34.32
ATOM	562	C	LEU	115	30.277	11.905	37.407	1.00	33.66
ATOM	563	O	LEU	115	29.359	12.718	37.563	1.00	34.73
ATOM	558	CB	LEU	115	29.506	10.127	35.928	1.00	34.23
ATOM	559	CG	LEU	115	29.644	8.789	35.224	1.00	35.32
ATOM	560	CD1	LEU	115	29.081	8.998	33.854	1.00	42.43
ATOM	561	CD2	LEU	115	31.081	8.349	35.070	1.00	37.40
ATOM	564	N	GLN	116	31.526	12.280	37.185	1.00	33.52
ATOM	565	CA	GLN	116	31.879	13.681	37.251	1.00	35.48
ATOM	571	C	GLN	116	31.537	14.466	36.017	1.00	33.45
ATOM	572	O	GLN	116	31.712	14.014	34.903	1.00	27.20
ATOM	566	CB	GLN	116	33.358	13.860	37.588	1.00	44.39
ATOM	567	CG	GLN	116	33.613	13.519	39.058	1.00	55.49
ATOM	568	CD	GLN	116	34.925	14.025	39.615	1.00	61.22
ATOM	569	OE1	GLN	116	35.991	13.915	38.973	1.00	66.18
ATOM	570	NE2	GLN	116	34.867	14.565	40.833	1.00	58.06
ATOM	573	N	PRO	117	30.986	15.650	36.210	1.00	33.36
ATOM	575	CA	PRO	117	30.610	16.530	35.118	1.00	35.10
ATOM	578	C	PRO	117	31.812	16.869	34.290	1.00	33.92
ATOM	579	O	PRO	117	32.863	17.135	34.831	1.00	39.00
ATOM	576	CB	PRO	117	30.118	17.752	35.852	1.00	31.85
ATOM	577	CG	PRO	117	29.403	17.130	36.955	1.00	38.23
ATOM	574	CD	PRO	117	30.370	16.093	37.454	1.00	35.43
ATOM	580	N	ASP	118	31.675	16.773	32.976	1.00	34.87
ATOM	581	CA	ASP	118	32.745	17.109	32.048	1.00	31.79
ATOM	586	C	ASP	118	32.011	17.810	30.934	1.00	29.11
ATOM	587	O	ASP	118	31.477	17.163	30.058	1.00	32.62
ATOM	582	CB	ASP	118	33.445	15.852	31.534	1.00	27.53

Fig. 21L

ATOM	583	CG	ASP	118	34.835	16.144	30.937	1.00	29.42
ATOM	584	OD1	ASP	118	35.038	17.178	30.258	1.00	29.54
ATOM	585	OD2	ASP	118	35.730	15.301	31.120	1.00	30.32
ATOM	588	N	LYS	119	31.855	19.118	31.066	1.00	26.70
ATOM	589	CA	LYS	119	31.143	19.911	30.077	1.00	27.57
ATOM	595	C	LYS	119	31.510	19.643	28.619	1.00	25.98
ATOM	596	O	LYS	119	30.631	19.455	27.795	1.00	27.96
ATOM	590	CB	LYS	119	31.306	21.384	30.379	1.00	30.48
ATOM	591	CG	LYS	119	30.348	21.887	31.415	1.00	41.34
ATOM	592	CD	LYS	119	30.650	23.345	31.784	1.00	46.39
ATOM	593	CE	LYS	119	29.436	24.017	32.460	1.00	54.46
ATOM	594	NZ	LYS	119	28.938	23.380	33.740	1.00	57.23
ATOM	597	N	VAL	120	32.800	19.632	28.301	1.00	22.59
ATOM	598	CA	VAL	120	33.259	19.376	26.944	1.00	16.79
ATOM	602	C	VAL	120	32.995	17.921	26.532	1.00	20.68
ATOM	603	O	VAL	120	32.563	17.666	25.414	1.00	24.32
ATOM	599	CB	VAL	120	34.757	19.651	26.813	1.00	15.66
ATOM	600	CG1	VAL	120	35.210	19.423	25.386	1.00	14.04
ATOM	601	CG2	VAL	120	35.066	21.054	27.256	1.00	12.50
ATOM	604	N	VAL	121	33.249	16.962	27.425	1.00	20.59
ATOM	605	CA	VAL	121	33.023	15.559	27.099	1.00	15.94
ATOM	609	C	VAL	121	31.541	15.290	26.866	1.00	23.12
ATOM	610	O	VAL	121	31.175	14.388	26.091	1.00	27.04
ATOM	606	CB	VAL	121	33.604	14.614	28.176	1.00	13.62
ATOM	607	CG1	VAL	121	33.111	13.206	28.002	1.00	16.87
ATOM	608	CG2	VAL	121	35.104	14.588	28.115	1.00	12.10
ATOM	611	N	GLU	122	30.691	16.147	27.430	1.00	22.34
ATOM	612	CA	GLU	122	29.258	15.969	27.316	1.00	17.82
ATOM	618	C	GLU	122	28.692	16.753	26.182	1.00	20.51
ATOM	619	O	GLU	122	27.624	16.445	25.660	1.00	20.42
ATOM	613	CB	GLU	122	28.574	16.361	28.598	1.00	21.95
ATOM	614	CG	GLU	122	28.841	15.460	29.765	1.00	27.87
ATOM	615	CD	GLU	122	28.146	15.985	31.001	1.00	36.96
ATOM	616	OE1	GLU	122	26.893	15.854	31.101	1.00	31.07
ATOM	617	OE2	GLU	122	28.850	16.586	31.843	1.00	39.15
ATOM	620	N	PHE	123	29.345	17.830	25.823	1.00	19.09
ATOM	621	CA	PHE	123	28.819	18.535	24.680	1.00	19.82
ATOM	629	C	PHE	123	29.111	17.634	23.484	1.00	19.97
ATOM	630	O	PHE	123	28.271	17.430	22.625	1.00	20.96
ATOM	622	CB	PHE	123	29.518	19.857	24.495	1.00	20.90
ATOM	623	CG	PHE	123	29.026	20.604	23.355	1.00	18.92
ATOM	624	CD1	PHE	123	27.909	21.400	23.482	1.00	18.73
ATOM	625	CD2	PHE	123	29.661	20.511	22.139	1.00	22.28
ATOM	626	CE1	PHE	123	27.429	22.103	22.398	1.00	22.70
ATOM	627	CE2	PHE	123	29.183	21.213	21.048	1.00	24.76
ATOM	628	CZ	PHE	123	28.069	22.010	21.178	1.00	19.92
ATOM	631	N	LEU	124	30.312	17.069	23.448	1.00	21.40
ATOM	632	CA	LEU	124	30.688	16.176	22.365	1.00	17.35
ATOM	637	C	LEU	124	29.731	15.001	22.304	1.00	17.32
ATOM	638	O	LEU	124	29.092	14.816	21.289	1.00	21.33
ATOM	633	CB	LEU	124	32.111	15.695	22.547	1.00	17.34
ATOM	634	CG	LEU	124	33.165	16.769	22.368	1.00	19.10
ATOM	635	CD1	LEU	124	34.533	16.195	22.690	1.00	23.46
ATOM	636	CD2	LEU	124	33.124	17.265	20.940	1.00	21.60

Fig. 21M

ATOM	639	N	SER	125	29.514	14.303	23.422	1.00	19.23
ATOM	640	CA	SER	125	28.614	13.135	23.444	1.00	19.37
ATOM	643	C	SER	125	27.198	13.399	22.963	1.00	20.02
ATOM	644	O	SER	125	26.555	12.511	22.453	1.00	26.02
ATOM	641	CB	SER	125	28.564	12.477	24.831	1.00	15.49
ATOM	642	OG	SER	125	29.862	12.341	25.357	1.00	17.39
ATOM	645	N	GLY	126	26.685	14.587	23.186	1.00	22.04
ATOM	646	CA	GLY	126	25.346	14.897	22.748	1.00	22.04
ATOM	647	C	GLY	126	25.311	15.508	21.354	1.00	26.13
ATOM	648	O	GLY	126	24.225	15.563	20.761	1.00	30.84
ATOM	649	N	SER	127	26.444	16.034	20.867	1.00	23.79
ATOM	650	CA	SER	127	26.525	16.611	19.513	1.00	25.27
ATOM	653	C	SER	127	26.940	15.600	18.457	1.00	25.87
ATOM	654	O	SER	127	26.228	15.412	17.478	1.00	29.17
ATOM	651	CB	SER	127	27.536	17.731	19.434	1.00	19.35
ATOM	652	OG	SER	127	27.123	18.782	20.249	1.00	34.49
ATOM	655	N	TYR	128	28.109	14.992	18.653	1.00	17.70
ATOM	656	CA	TYR	128	28.687	14.042	17.725	1.00	16.14
ATOM	665	C	TYR	128	28.584	12.627	18.236	1.00	16.55
ATOM	666	O	TYR	128	29.593	11.963	18.448	1.00	19.42
ATOM	657	CB	TYR	128	30.151	14.425	17.497	1.00	13.00
ATOM	658	CG	TYR	128	30.260	15.848	17.059	1.00	10.30
ATOM	659	CD1	TYR	128	29.527	16.303	15.979	1.00	12.91
ATOM	661	CD2	TYR	128	30.973	16.763	17.803	1.00	14.08
ATOM	660	CE1	TYR	128	29.484	17.631	15.672	1.00	17.29
ATOM	662	CE2	TYR	128	30.945	18.103	17.511	1.00	16.38
ATOM	663	CZ	TYR	128	30.186	18.541	16.440	1.00	20.39
ATOM	664	OH	TYR	128	30.098	19.905	16.162	1.00	22.10
ATOM	667	N	ALA	129	27.371	12.118	18.261	1.00	11.21
ATOM	668	CA	ALA	129	27.108	10.806	18.820	1.00	14.30
ATOM	670	C	ALA	129	27.356	9.563	18.033	1.00	15.80
ATOM	671	O	ALA	129	26.860	8.510	18.419	1.00	15.01
ATOM	669	CB	ALA	129	25.685	10.769	19.310	1.00	13.72
ATOM	672	N	GLY	130	28.004	9.660	16.885	1.00	21.28
ATOM	673	CA	GLY	130	28.225	8.453	16.091	1.00	22.57
ATOM	674	C	GLY	130	29.478	8.536	15.252	1.00	21.76
ATOM	675	O	GLY	130	29.926	9.616	14.966	1.00	25.44
ATOM	676	N	LEU	131	30.051	7.416	14.865	1.00	22.99
ATOM	677	CA	LEU	131	31.246	7.417	14.042	1.00	26.31
ATOM	682	C	LEU	131	30.994	6.854	12.641	1.00	29.53
ATOM	683	O	LEU	131	30.034	6.085	12.406	1.00	26.35
ATOM	678	CB	LEU	131	32.346	6.580	14.714	1.00	20.02
ATOM	679	CG	LEU	131	32.891	7.044	16.055	1.00	20.16
ATOM	680	CD1	LEU	131	33.596	5.914	16.648	1.00	16.69
ATOM	681	CD2	LEU	131	33.839	8.224	15.937	1.00	18.57
ATOM	684	N	SER	132	31.789	7.324	11.685	1.00	31.91
ATOM	685	CA	SER	132	31.684	6.775	10.342	1.00	35.56
ATOM	688	C	SER	132	32.998	6.895	9.665	1.00	30.11
ATOM	689	O	SER	132	33.732	7.815	9.895	1.00	33.36
ATOM	686	CB	SER	132	30.507	7.294	9.522	1.00	40.11
ATOM	687	OG	SER	132	30.763	8.505	8.839	1.00	48.47
ATOM	690	N	LEU	133	33.377	5.799	9.063	1.00	35.05
ATOM	691	CA	LEU	133	34.657	5.623	8.399	1.00	35.32
ATOM	696	C	LEU	133	34.518	5.939	6.938	1.00	40.82

Fig. 21N

ATOM	697	O	LEU	133	33.563	5.480	6.310	1.00	44.46
ATOM	692	CB	LEU	133	35.005	4.158	8.562	1.00	26.30
ATOM	693	CG	LEU	133	36.158	3.559	7.859	1.00	19.38
ATOM	694	CD1	LEU	133	37.423	4.183	8.304	1.00	26.92
ATOM	695	CD2	LEU	133	36.143	2.131	8.217	1.00	25.27
ATOM	698	N	SER	134	35.438	6.734	6.395	1.00	44.63
ATOM	699	CA	SER	134	35.414	7.089	4.971	1.00	45.92
ATOM	702	C	SER	134	36.666	6.529	4.271	1.00	47.21
ATOM	703	O	SER	134	37.802	6.751	4.720	1.00	44.61
ATOM	700	CB	SER	134	35.326	8.598	4.795	1.00	45.63
ATOM	701	OG	SER	134	36.609	9.183	4.988	1.00	47.82
ATOM	704	N	SER	135	36.451	5.756	3.209	1.00	49.21
ATOM	705	CA	SER	135	37.548	5.179	2.467	1.00	51.54
ATOM	708	C	SER	135	37.797	5.987	1.220	1.00	53.51
ATOM	709	O	SER	135	37.042	6.906	0.907	1.00	54.49
ATOM	706	CB	SER	135	37.225	3.744	2.104	1.00	52.24
ATOM	707	OG	SER	135	37.043	2.974	3.275	1.00	62.08
ATOM	710	N	ARG	136	38.873	5.665	0.516	1.00	55.26
ATOM	711	CA	ARG	136	39.191	6.373	-0.710	1.00	56.10
ATOM	714	C	ARG	136	38.326	5.886	-1.904	1.00	59.66
ATOM	715	O	ARG	136	37.840	4.744	-1.914	1.00	61.20
ATOM	712	CB	ARG	136	40.681	6.217	-0.998	1.00	55.37
ATOM	713	CG	ARG	136	41.445	6.949	-0.063	1.00	51.86
ATOM	716	N	ARG	137	38.080	6.785	-2.865	1.00	61.93
ATOM	717	CA	ARG	137	37.315	6.488	-4.090	1.00	60.62
ATOM	719	C	ARG	137	38.106	7.023	-5.321	1.00	61.32
ATOM	720	O	ARG	137	38.993	7.886	-5.178	1.00	60.21
ATOM	718	CB	ARG	137	35.913	7.129	-4.020	1.00	60.06
ATOM	721	N	CYS	138	37.849	6.460	-6.505	1.00	62.66
ATOM	722	CA	CYS	138	38.523	6.910	-7.739	1.00	63.23
ATOM	725	C	CYS	138	37.849	8.192	-8.210	1.00	62.65
ATOM	726	O	CYS	138	38.416	8.969	-8.974	1.00	61.75
ATOM	723	CB	CYS	138	38.414	5.853	-8.829	1.00	62.56
ATOM	724	SG	CYS	138	37.074	4.671	-8.542	1.00	69.15
ATOM	727	N	ASP	139	36.638	8.393	-7.695	1.00	62.87
ATOM	728	CA	ASP	139	35.800	9.554	-7.968	1.00	60.63
ATOM	733	C	ASP	139	36.354	10.873	-7.344	1.00	60.68
ATOM	734	O	ASP	139	36.365	11.921	-7.996	1.00	61.62
ATOM	729	CB	ASP	139	34.394	9.247	-7.389	1.00	59.02
ATOM	730	CG	ASP	139	33.267	10.106	-8.015	1.00	64.92
ATOM	731	OD1	ASP	139	33.541	11.238	-8.500	1.00	67.71
ATOM	732	OD2	ASP	139	32.078	9.653	-8.013	1.00	68.40
ATOM	735	N	ASP	140	36.881	10.798	-6.120	1.00	59.87
ATOM	736	CA	ASP	140	37.326	11.986	-5.381	1.00	59.86
ATOM	738	C	ASP	140	38.554	12.865	-5.756	1.00	59.66
ATOM	739	O	ASP	140	39.593	12.383	-6.241	1.00	61.53
ATOM	737	CB	ASP	140	37.304	11.676	-3.888	1.00	60.15
ATOM	740	N	VAL	141	38.401	14.169	-5.499	1.00	58.35
ATOM	741	CA	VAL	141	39.413	15.202	-5.788	1.00	60.08
ATOM	745	C	VAL	141	40.702	14.983	-4.989	1.00	62.62
ATOM	746	O	VAL	141	40.638	14.650	-3.802	1.00	67.89
ATOM	742	CB	VAL	141	38.853	16.621	-5.417	1.00	59.22
ATOM	743	CG1	VAL	141	39.882	17.695	-5.689	1.00	55.88
ATOM	744	CG2	VAL	141	37.561	16.900	-6.168	1.00	57.15

Fig. 210

ATOM	747	N	GLU	142	41.868	15.220	-5.582	1.00	61.91
ATOM	748	CA	GLU	142	43.106	15.032	-4.815	1.00	60.70
ATOM	750	C	GLU	142	44.159	16.169	-4.993	1.00	62.01
ATOM	751	O	GLU	142	44.385	16.613	-6.147	1.00	64.58
ATOM	749	CB	GLU	142	43.698	13.657	-5.121	1.00	61.45
ATOM	756	N	PRO	154	39.096	0.505	5.789	1.00	59.89
ATOM	757	CA	PRO	154	39.598	1.565	6.749	1.00	64.46
ATOM	754	C	PRO	154	40.569	2.451	5.968	1.00	65.07
ATOM	755	O	PRO	154	41.741	2.063	5.878	1.00	69.33
ATOM	753	CB	PRO	154	40.354	0.888	7.938	1.00	59.84
ATOM	758	N	PHE	155	40.159	3.636	5.468	1.00	62.65
ATOM	759	CA	PHE	155	41.101	4.423	4.614	1.00	58.28
ATOM	761	C	PHE	155	41.211	5.936	4.677	1.00	53.77
ATOM	762	O	PHE	155	42.109	6.472	5.289	1.00	54.45
ATOM	760	CB	PHE	155	40.956	3.984	3.105	1.00	59.87
ATOM	763	N	LYS	156	40.317	6.635	4.012	1.00	49.59
ATOM	764	CA	LYS	156	40.409	8.071	3.960	1.00	45.31
ATOM	770	C	LYS	156	40.452	8.808	5.294	1.00	41.39
ATOM	771	O	LYS	156	41.325	9.654	5.500	1.00	41.85
ATOM	765	CB	LYS	156	39.319	8.619	3.037	1.00	47.60
ATOM	766	CG	LYS	156	39.648	9.918	2.354	1.00	46.63
ATOM	767	CD	LYS	156	38.385	10.634	1.945	1.00	45.66
ATOM	768	CE	LYS	156	37.593	9.760	1.025	1.00	48.31
ATOM	769	NZ	LYS	156	36.171	10.159	1.042	1.00	56.75
ATOM	772	N	HIS	157	39.546	8.501	6.209	1.00	38.72
ATOM	773	CA	HIS	157	39.519	9.209	7.509	1.00	37.81
ATOM	774	C	HIS	157	38.351	8.715	8.340	1.00	36.09
ATOM	775	O	HIS	157	37.580	7.867	7.857	1.00	38.87
ATOM	776	CB	HIS	157	39.330	10.731	7.318	1.00	37.59
ATOM	777	CG	HIS	157	38.004	11.116	6.696	1.00	36.75
ATOM	778	ND1	HIS	157	37.866	11.849	5.537	1.00	36.56
ATOM	779	CD2	HIS	157	36.735	10.827	7.089	1.00	34.55
ATOM	781	CE1	HIS	157	36.557	11.960	5.284	1.00	31.88
ATOM	780	NE2	HIS	157	35.838	11.354	6.207	1.00	31.66
ATOM	782	N	VAL	158	38.186	9.258	9.559	1.00	34.03
ATOM	783	CA	VAL	158	37.058	8.911	10.434	1.00	30.28
ATOM	787	C	VAL	158	36.395	10.219	10.823	1.00	25.84
ATOM	788	O	VAL	158	37.081	11.185	11.182	1.00	23.69
ATOM	784	CB	VAL	158	37.441	8.114	11.731	1.00	31.15
ATOM	785	CG1	VAL	158	36.168	7.750	12.475	1.00	31.88
ATOM	786	CG2	VAL	158	38.151	6.814	11.410	1.00	22.16
ATOM	789	N	ALA	159	35.073	10.240	10.741	1.00	22.52
ATOM	790	CA	ALA	159	34.318	11.434	11.027	1.00	23.37
ATOM	792	C	ALA	159	33.428	11.278	12.244	1.00	25.14
ATOM	793	O	ALA	159	32.971	10.174	12.539	1.00	24.28
ATOM	791	CB	ALA	159	33.448	11.737	9.841	1.00	25.21
ATOM	794	N	LEU	160	33.199	12.380	12.954	1.00	26.27
ATOM	795	CA	LEU	160	32.311	12.404	14.121	1.00	23.20
ATOM	800	C	LEU	160	31.013	12.946	13.556	1.00	23.47
ATOM	801	O	LEU	160	31.009	14.018	12.979	1.00	20.58
ATOM	796	CB	LEU	160	32.808	13.360	15.198	1.00	27.37
ATOM	797	CG	LEU	160	34.203	13.205	15.810	1.00	31.90
ATOM	798	CD1	LEU	160	34.298	14.188	17.009	1.00	33.23
ATOM	799	CD2	LEU	160	34.462	11.745	16.248	1.00	26.75

Fig. 21P

ATOM	802	N	CYS	161	29.916	12.237	13.777	1.00	23.74
ATOM	803	CA	CYS	161	28.631	12.615	13.223	1.00	26.80
ATOM	806	C	CYS	161	27.518	12.672	14.261	1.00	25.72
ATOM	807	O	CYS	161	27.665	12.141	15.362	1.00	30.63
ATOM	804	CB	CYS	161	28.229	11.576	12.177	1.00	31.50
ATOM	805	SG	CYS	161	29.544	11.000	11.196	1.00	35.88
ATOM	808	N	SER	162	26.366	13.206	13.868	1.00	24.30
ATOM	809	CA	SER	162	25.236	13.319	14.773	1.00	27.46
ATOM	812	C	SER	162	24.841	11.971	15.162	1.00	25.69
ATOM	813	O	SER	162	24.443	11.737	16.281	1.00	30.53
ATOM	810	CB	SER	162	24.037	13.949	14.098	1.00	29.54
ATOM	811	OG	SER	162	24.203	15.333	14.021	1.00	40.86
ATOM	814	N	VAL	163	24.894	11.109	14.174	1.00	26.40
ATOM	815	CA	VAL	163	24.533	9.720	14.310	1.00	30.19
ATOM	819	C	VAL	163	25.192	9.012	13.105	1.00	32.44
ATOM	820	O	VAL	163	25.279	9.593	12.013	1.00	37.05
ATOM	816	CB	VAL	163	22.981	9.574	14.346	1.00	24.63
ATOM	817	CG1	VAL	163	22.349	10.183	13.084	1.00	26.16
ATOM	818	CG2	VAL	163	22.601	8.131	14.532	1.00	19.95
ATOM	821	N	GLY	164	25.813	7.860	13.340	1.00	32.29
ATOM	822	CA	GLY	164	26.454	7.136	12.251	1.00	31.63
ATOM	823	C	GLY	164	25.442	6.526	11.307	1.00	33.63
ATOM	824	O	GLY	164	24.249	6.573	11.563	1.00	33.91
ATOM	825	N	ARG	165	25.889	5.958	10.199	1.00	38.58
ATOM	826	CA	ARG	165	24.933	5.344	9.268	1.00	42.05
ATOM	828	C	ARG	165	24.799	3.848	9.555	1.00	41.87
ATOM	829	O	ARG	165	23.693	3.301	9.630	1.00	45.87
ATOM	827	CB	ARG	165	25.351	5.595	7.809	1.00	43.59
ATOM	830	N	ARG	166	25.937	3.178	9.667	1.00	42.35
ATOM	831	CA	ARG	166	25.960	1.765	9.989	1.00	42.46
ATOM	839	C	ARG	166	25.579	1.750	11.467	1.00	41.38
ATOM	840	O	ARG	166	25.946	2.659	12.217	1.00	42.45
ATOM	832	CB	ARG	166	27.367	1.218	9.784	1.00	47.34
ATOM	833	CG	ARG	166	27.620	0.620	8.421	1.00	52.97
ATOM	834	CD	ARG	166	29.030	0.082	8.331	1.00	56.09
ATOM	835	NE	ARG	166	29.974	1.193	8.297	1.00	60.10
ATOM	836	CZ	ARG	166	30.849	1.394	7.307	1.00	65.05
ATOM	837	NH1	ARG	166	30.922	0.527	6.286	1.00	66.02
ATOM	838	NH2	ARG	166	31.671	2.447	7.335	1.00	62.96
ATOM	841	N	ARG	167	24.813	0.759	11.889	1.00	41.55
ATOM	842	CA	ARG	167	24.375	0.702	13.286	1.00	42.74
ATOM	844	C	ARG	167	25.433	0.164	14.269	1.00	40.29
ATOM	845	O	ARG	167	26.283	-0.625	13.868	1.00	41.10
ATOM	843	CB	ARG	167	23.062	-0.082	13.387	1.00	45.33
ATOM	846	N	GLY	168	25.461	0.714	15.488	1.00	35.52
ATOM	847	CA	GLY	168	26.408	0.281	16.515	1.00	33.40
ATOM	848	C	GLY	168	27.646	1.167	16.588	1.00	32.69
ATOM	849	O	GLY	168	28.575	0.949	17.371	1.00	36.01
ATOM	850	N	THR	169	27.629	2.208	15.769	1.00	30.93
ATOM	851	CA	THR	169	28.703	3.166	15.661	1.00	26.29
ATOM	855	C	THR	169	28.481	4.322	16.633	1.00	26.10
ATOM	856	O	THR	169	28.599	5.478	16.259	1.00	24.59
ATOM	852	CB	THR	169	28.731	3.726	14.247	1.00	28.83
ATOM	853	OG1	THR	169	27.392	4.105	13.879	1.00	28.62

Fig. 21Q

ATOM	854	CG2	THR	169	29.260	2.693	13.253	1.00	27.89
ATOM	857	N	LEU	170	28.141	4.015	17.880	1.00	24.07
ATOM	858	CA	LEU	170	27.934	5.052	18.887	1.00	22.26
ATOM	863	C	LEU	170	29.286	5.582	19.351	1.00	23.34
ATOM	864	O	LEU	170	30.203	4.815	19.545	1.00	30.30
ATOM	859	CB	LEU	170	27.205	4.444	20.076	1.00	17.79
ATOM	860	CG	LEU	170	26.781	5.322	21.245	1.00	22.14
ATOM	861	CD1	LEU	170	25.593	6.188	20.856	1.00	22.03
ATOM	862	CD2	LEU	170	26.344	4.410	22.332	1.00	17.91
ATOM	865	N	ALA	171	29.458	6.880	19.501	1.00	22.71
ATOM	866	CA	ALA	171	30.738	7.359	19.999	1.00	18.39
ATOM	868	C	ALA	171	30.687	7.505	21.546	1.00	21.02
ATOM	869	O	ALA	171	29.669	7.937	22.113	1.00	24.45
ATOM	867	CB	ALA	171	31.107	8.673	19.325	1.00	19.01
ATOM	870	N	VAL	172	31.764	7.105	22.225	1.00	21.22
ATOM	871	CA	VAL	172	31.871	7.174	23.687	1.00	16.73
ATOM	875	C	VAL	172	33.089	8.042	23.944	1.00	16.31
ATOM	876	O	VAL	172	34.175	7.668	23.544	1.00	22.44
ATOM	872	CB	VAL	172	32.124	5.746	24.260	1.00	18.77
ATOM	873	CG1	VAL	172	32.502	5.781	25.716	1.00	19.85
ATOM	874	CG2	VAL	172	30.920	4.879	24.038	1.00	16.80
ATOM	877	N	TYR	173	32.916	9.229	24.515	1.00	14.11
ATOM	878	CA	TYR	173	34.047	10.104	24.754	1.00	12.78
ATOM	887	C	TYR	173	34.509	9.924	26.161	1.00	19.84
ATOM	888	O	TYR	173	33.749	9.519	27.027	1.00	20.82
ATOM	879	CB	TYR	173	33.672	11.563	24.533	1.00	15.57
ATOM	880	CG	TYR	173	33.296	11.895	23.101	1.00	17.92
ATOM	881	CD1	TYR	173	32.074	11.481	22.575	1.00	18.64
ATOM	883	CD2	TYR	173	34.176	12.567	22.257	1.00	17.47
ATOM	882	CE1	TYR	173	31.738	11.726	21.252	1.00	17.54
ATOM	884	CE2	TYR	173	33.850	12.803	20.932	1.00	17.35
ATOM	885	CZ	TYR	173	32.625	12.381	20.433	1.00	17.84
ATOM	886	OH	TYR	173	32.264	12.598	19.116	1.00	16.93
ATOM	889	N	GLY	174	35.757	10.257	26.417	1.00	22.64
ATOM	890	CA	GLY	174	36.290	10.079	27.741	1.00	23.42
ATOM	891	C	GLY	174	37.567	10.851	27.832	1.00	24.50
ATOM	892	O	GLY	174	37.989	11.411	26.851	1.00	29.56
ATOM	893	N	ARG	175	38.143	10.967	29.015	1.00	27.20
ATOM	894	CA	ARG	175	39.384	11.705	29.153	1.00	29.49
ATOM	902	C	ARG	175	40.534	10.730	29.228	1.00	31.91
ATOM	903	O	ARG	175	41.688	11.114	29.142	1.00	32.67
ATOM	895	CB	ARG	175	39.330	12.543	30.409	1.00	27.65
ATOM	896	CG	ARG	175	38.413	13.722	30.282	1.00	29.67
ATOM	897	CD	ARG	175	38.972	14.827	29.325	1.00	30.15
ATOM	898	NE	ARG	175	38.059	15.959	29.362	1.00	31.04
ATOM	899	CZ	ARG	175	38.234	17.120	28.755	1.00	34.65
ATOM	900	NH1	ARG	175	39.338	17.370	28.046	1.00	30.78
ATOM	901	NH2	ARG	175	37.282	18.040	28.888	1.00	37.65
ATOM	904	N	ASP	176	40.181	9.450	29.248	1.00	35.20
ATOM	905	CA	ASP	176	41.124	8.363	29.359	1.00	32.03
ATOM	910	C	ASP	176	40.893	7.233	28.315	1.00	30.86
ATOM	911	O	ASP	176	39.787	6.749	28.121	1.00	31.67
ATOM	906	CB	ASP	176	40.936	7.827	30.759	1.00	39.47
ATOM	907	CG	ASP	176	42.002	6.886	31.161	1.00	48.38

Fig. 21R

ATOM	908	OD1	ASP	176	41.984	5.705	30.744	1.00	50.80
ATOM	909	OD2	ASP	176	42.863	7.338	31.928	1.00	58.97
ATOM	912	N	PRO	177	41.951	6.787	27.640	1.00	29.45
ATOM	914	CA	PRO	177	41.797	5.717	26.652	1.00	30.26
ATOM	917	C	PRO	177	41.423	4.366	27.241	1.00	30.24
ATOM	918	O	PRO	177	40.773	3.557	26.598	1.00	35.30
ATOM	915	CB	PRO	177	43.159	5.681	25.961	1.00	31.05
ATOM	916	CG	PRO	177	44.096	6.266	26.973	1.00	31.34
ATOM	913	CD	PRO	177	43.296	7.379	27.574	1.00	30.42
ATOM	919	N	GLU	178	41.883	4.067	28.439	1.00	30.89
ATOM	920	CA	GLU	178	41.501	2.803	29.038	1.00	28.04
ATOM	926	C	GLU	178	40.036	2.907	29.458	1.00	25.53
ATOM	927	O	GLU	178	39.242	2.048	29.157	1.00	28.11
ATOM	921	CB	GLU	178	42.349	2.501	30.268	1.00	30.41
ATOM	922	CG	GLU	178	42.096	1.118	30.858	1.00	32.44
ATOM	923	CD	GLU	178	42.790	0.050	30.058	1.00	37.09
ATOM	924	OE1	GLU	178	43.951	0.283	29.671	1.00	41.06
ATOM	925	OE2	GLU	178	42.204	-1.024	29.823	1.00	40.37
ATOM	928	N	TRP	179	39.671	4.004	30.087	1.00	20.27
ATOM	929	CA	TRP	179	38.324	4.155	30.549	1.00	18.02
ATOM	940	C	TRP	179	37.368	4.024	29.387	1.00	24.92
ATOM	941	O	TRP	179	36.320	3.383	29.496	1.00	29.25
ATOM	930	CB	TRP	179	38.144	5.495	31.248	1.00	11.02
ATOM	931	CG	TRP	179	36.823	5.629	31.885	1.00	20.08
ATOM	935	CD1	TRP	179	36.465	5.170	33.139	1.00	15.42
ATOM	932	CD2	TRP	179	35.650	6.286	31.341	1.00	20.80
ATOM	936	NE1	TRP	179	35.158	5.508	33.392	1.00	21.65
ATOM	933	CE2	TRP	179	34.632	6.193	32.314	1.00	19.89
ATOM	934	CE3	TRP	179	35.363	6.944	30.131	1.00	17.76
ATOM	937	CZ2	TRP	179	33.332	6.743	32.114	1.00	21.72
ATOM	938	CZ3	TRP	179	34.088	7.478	29.933	1.00	14.57
ATOM	939	CH2	TRP	179	33.080	7.374	30.929	1.00	16.92
ATOM	942	N	VAL	180	37.735	4.585	28.247	1.00	24.63
ATOM	943	CA	VAL	180	36.856	4.494	27.095	1.00	24.07
ATOM	947	C	VAL	180	36.723	3.096	26.522	1.00	27.82
ATOM	948	O	VAL	180	35.628	2.668	26.159	1.00	30.00
ATOM	944	CB	VAL	180	37.320	5.411	25.990	1.00	23.26
ATOM	945	CG1	VAL	180	36.454	5.201	24.706	1.00	15.40
ATOM	946	CG2	VAL	180	37.321	6.832	26.513	1.00	22.46
ATOM	949	N	THR	181	37.837	2.383	26.415	1.00	30.50
ATOM	950	CA	THR	181	37.795	1.047	25.838	1.00	32.25
ATOM	954	C	THR	181	37.092	0.171	26.810	1.00	30.35
ATOM	955	O	THR	181	36.368	-0.746	26.445	1.00	31.45
ATOM	951	CB	THR	181	39.208	0.499	25.525	1.00	34.34
ATOM	952	OG1	THR	181	40.040	0.576	26.690	1.00	38.46
ATOM	953	CG2	THR	181	39.851	1.350	24.410	1.00	38.81
ATOM	956	N	GLN	182	37.181	0.582	28.057	1.00	29.82
ATOM	957	CA	GLN	182	36.595	-0.167	29.133	1.00	29.92
ATOM	963	C	GLN	182	35.066	-0.110	29.197	1.00	29.67
ATOM	964	O	GLN	182	34.452	-0.954	29.835	1.00	32.79
ATOM	958	CB	GLN	182	37.226	0.292	30.441	1.00	27.17
ATOM	959	CG	GLN	182	37.224	-0.750	31.488	1.00	32.42
ATOM	960	CD	GLN	182	38.447	-1.608	31.550	1.00	29.47
ATOM	961	OE1	GLN	182	38.348	-2.785	31.833	1.00	36.45

Fig. 21S

ATOM	962	NE2	GLN	182	39.603	-1.022	31.372	1.00	33.03
ATOM	965	N	ARG	183	34.435	0.853	28.532	1.00	27.46
ATOM	966	CA	ARG	183	32.973	0.935	28.588	1.00	24.82
ATOM	974	C	ARG	183	32.275	-0.096	27.725	1.00	23.34
ATOM	975	O	ARG	183	31.073	-0.235	27.816	1.00	27.80
ATOM	967	CB	ARG	183	32.450	-2.306	28.115	1.00	23.83
ATOM	968	CG	ARG	183	33.142	3.513	28.631	1.00	22.14
ATOM	969	CD	ARG	183	32.896	3.677	30.118	1.00	27.34
ATOM	970	NE	ARG	183	34.006	3.109	30.870	1.00	27.57
ATOM	971	CZ	ARG	183	33.956	2.723	32.136	1.00	24.93
ATOM	972	NH1	ARG	183	32.841	2.809	32.848	1.00	25.63
ATOM	973	NH2	ARG	183	35.040	2.222	32.676	1.00	26.19
ATOM	976	N	PHE	184	33.012	-0.762	26.846	1.00	23.74
ATOM	977	CA	PHE	184	32.445	-1.705	25.879	1.00	21.79
ATOM	985	C	PHE	184	32.474	-3.168	26.272	1.00	25.02
ATOM	986	O	PHE	184	33.533	-3.767	26.196	1.00	30.09
ATOM	978	CB	PHE	184	33.187	-1.522	24.536	1.00	17.97
ATOM	979	CG	PHE	184	32.998	-0.161	23.935	1.00	16.79
ATOM	980	CD1	PHE	184	33.799	0.884	24.302	1.00	17.05
ATOM	981	CD2	PHE	184	31.947	0.087	23.067	1.00	18.31
ATOM	982	CE1	PHE	184	33.556	2.147	23.835	1.00	20.88
ATOM	983	CE2	PHE	184	31.699	1.346	22.597	1.00	15.11
ATOM	984	CZ	PHE	184	32.503	2.382	22.977	1.00	18.91
ATOM	987	N	PRO	185	31.317	-3.780	26.649	1.00	24.94
ATOM	989	CA	PRO	185	31.322	-5.193	27.030	1.00	25.81
ATOM	992	C	PRO	185	31.696	-6.230	25.951	1.00	29.32
ATOM	993	O	PRO	185	31.813	-7.418	26.267	1.00	34.66
ATOM	990	CB	PRO	185	29.919	-5.400	27.621	1.00	21.70
ATOM	991	CG	PRO	185	29.114	-4.417	26.970	1.00	22.66
ATOM	988	CD	PRO	185	30.003	-3.199	26.969	1.00	23.75
ATOM	994	N	ASP	186	31.866	-5.816	24.692	1.00	30.88
ATOM	995	CA	ASP	186	32.298	-6.762	23.629	1.00	33.49
ATOM	1000	C	ASP	186	33.833	-6.863	23.706	1.00	35.14
ATOM	1001	O	ASP	186	34.437	-7.773	23.144	1.00	37.18
ATOM	996	CB	ASP	186	31.995	-6.276	22.190	1.00	29.65
ATOM	997	CG	ASP	186	30.738	-5.487	22.078	1.00	34.74
ATOM	998	OD1	ASP	186	30.761	-4.272	22.431	1.00	43.46
ATOM	999	OD2	ASP	186	29.725	-6.058	21.618	1.00	33.67
ATOM	1002	N	LEU	187	34.453	-5.834	24.284	1.00	33.94
ATOM	1003	CA	LEU	187	35.892	-5.748	24.401	1.00	29.03
ATOM	1008	C	LEU	187	36.498	-6.582	25.490	1.00	28.92
ATOM	1009	O	LEU	187	36.361	-6.317	26.675	1.00	37.06
ATOM	1004	CB	LEU	187	36.307	-4.296	24.542	1.00	29.47
ATOM	1005	CG	LEU	187	36.682	-3.573	23.249	1.00	27.53
ATOM	1006	CD1	LEU	187	35.599	-3.735	22.192	1.00	25.99
ATOM	1007	CD2	LEU	187	36.944	-2.133	23.571	1.00	22.13
ATOM	1010	N	THR	188	37.106	-7.652	25.051	1.00	27.92
ATOM	1011	CA	THR	188	37.803	-8.615	25.861	1.00	27.24
ATOM	1015	C	THR	188	39.100	-7.964	26.352	1.00	30.44
ATOM	1016	O	THR	188	39.565	-6.986	25.751	1.00	30.56
ATOM	1012	CB	THR	188	38.059	-9.822	24.940	1.00	24.35
ATOM	1013	OG1	THR	188	37.076	-10.819	25.204	1.00	30.69
ATOM	1014	CG2	THR	188	39.436	-10.381	25.027	1.00	28.27
ATOM	1017	N	ALA	189	39.686	-8.506	27.431	1.00	34.52

Fig. 21T

ATOM	1018	CA	ALA	189	40.944	-7.990	28.009	1.00	35.65
ATOM	1020	C	ALA	189	42.007	-8.011	26.946	1.00	39.97
ATOM	1021	O	ALA	189	42.881	-7.147	26.894	1.00	42.65
ATOM	1019	CB	ALA	189	41.375	-8.839	29.121	1.00	35.31
ATOM	1022	N	ALA	190	41.948	-9.064	26.139	1.00	40.80
ATOM	1023	CA	ALA	190	42.843	-9.253	25.017	1.00	39.84
ATOM	1025	C	ALA	190	42.728	-8.051	24.056	1.00	40.77
ATOM	1026	O	ALA	190	43.708	-7.351	23.806	1.00	43.57
ATOM	1024	CB	ALA	190	42.462	-10.519	24.310	1.00	38.24
ATOM	1027	N	ASP	191	41.519	-7.803	23.549	1.00	38.93
ATOM	1028	CA	ASP	191	41.273	-6.699	22.641	1.00	32.55
ATOM	1033	C	ASP	191	41.831	-5.499	23.249	1.00	33.63
ATOM	1034	O	ASP	191	42.509	-4.743	22.583	1.00	37.50
ATOM	1029	CB	ASP	191	39.799	-6.433	22.502	1.00	29.76
ATOM	1030	CG	ASP	191	39.073	-7.599	21.963	1.00	36.25
ATOM	1031	OD1	ASP	191	39.714	-8.479	21.341	1.00	41.09
ATOM	1032	OD2	ASP	191	37.852	-7.648	22.146	1.00	41.30
ATOM	1035	N	ARG	192	41.573	-5.324	24.539	1.00	34.17
ATOM	1036	CA	ARG	192	42.049	-4.126	25.195	1.00	37.71
ATOM	1044	C	ARG	192	43.566	-4.008	25.211	1.00	42.33
ATOM	1045	O	ARG	192	44.090	-2.895	25.317	1.00	43.93
ATOM	1037	CB	ARG	192	41.391	-3.928	26.578	1.00	36.86
ATOM	1038	CG	ARG	192	39.861	-3.690	26.511	1.00	27.25
ATOM	1039	CD	ARG	192	39.264	-3.248	27.835	1.00	30.69
ATOM	1040	NE	ARG	192	39.714	-4.055	28.972	1.00	35.90
ATOM	1041	CZ	ARG	192	39.097	-5.143	29.446	1.00	39.05
ATOM	1042	NH1	ARG	192	37.954	-5.583	28.909	1.00	36.96
ATOM	1043	NH2	ARG	192	39.628	-5.794	30.476	1.00	32.71
ATOM	1046	N	ASP	193	44.259	-5.139	25.013	1.00	45.77
ATOM	1047	CA	ASP	193	45.734	-5.193	24.966	1.00	45.44
ATOM	1052	C	ASP	193	46.270	-4.678	23.630	1.00	44.24
ATOM	1053	O	ASP	193	47.166	-3.814	23.590	1.00	45.99
ATOM	1048	CB	ASP	193	46.251	-6.625	25.186	1.00	48.79
ATOM	1049	CG	ASP	193	46.342	-7.006	26.647	1.00	50.37
ATOM	1050	OD1	ASP	193	46.423	-6.089	27.491	1.00	51.03
ATOM	1051	OD2	ASP	193	46.343	-8.224	26.941	1.00	48.61
ATOM	1054	N	GLY	194	45.752	-5.231	22.536	1.00	43.02
ATOM	1055	CA	GLY	194	46.187	-4.787	21.220	1.00	42.74
ATOM	1056	C	GLY	194	45.952	-3.300	21.026	1.00	39.80
ATOM	1057	O	GLY	194	46.736	-2.603	20.407	1.00	45.17
ATOM	1058	N	LEU	195	44.852	-2.823	21.577	1.00	38.61
ATOM	1059	CA	LEU	195	44.471	-1.441	21.507	1.00	36.07
ATOM	1064	C	LEU	195	45.421	-0.548	22.286	1.00	38.26
ATOM	1065	O	LEU	195	45.959	0.413	21.731	1.00	38.71
ATOM	1060	CB	LEU	195	43.068	-1.311	22.061	1.00	35.04
ATOM	1061	CG	LEU	195	42.029	-1.749	21.049	1.00	37.00
ATOM	1062	CD1	LEU	195	40.612	-1.784	21.636	1.00	32.88
ATOM	1063	CD2	LEU	195	42.116	-0.745	19.900	1.00	39.88
ATOM	1066	N	ARG	196	45.625	-0.874	23.567	1.00	36.24
ATOM	1067	CA	ARG	196	46.484	-0.112	24.466	1.00	33.52
ATOM	1075	C	ARG	196	47.887	-0.024	23.965	1.00	37.30
ATOM	1076	O	ARG	196	48.540	1.012	24.128	1.00	38.25
ATOM	1068	CB	ARG	196	46.472	-0.709	25.844	1.00	32.83
ATOM	1069	CG	ARG	196	47.459	-0.101	26.800	1.00	39.70

Fig. 210

ATOM	1070	CD	ARG	196	46.917	-0.087	28.214	1.00	48.58
ATOM	1071	NE	ARG	196	46.608	-1.421	28.743	1.00	57.95
ATOM	1072	CZ	ARG	196	45.447	-2.068	28.588	1.00	62.66
ATOM	1073	NH1	ARG	196	44.448	-1.520	27.897	1.00	66.54
ATOM	1074	NH2	ARG	196	45.260	-3.255	29.156	1.00	64.26
ATOM	1077	N	ALA	197	48.358	-1.125	23.383	1.00	40.28
ATOM	1078	CA	ALA	197	49.694	-1.214	22.783	1.00	43.97
ATOM	1080	C	ALA	197	49.869	-0.097	21.719	1.00	46.74
ATOM	1081	O	ALA	197	50.943	0.499	21.564	1.00	45.42
ATOM	1079	CB	ALA	197	49.840	-2.567	22.116	1.00	43.21
ATOM	1082	N	GLN	198	48.792	0.136	20.964	1.00	48.99
ATOM	1083	CA	GLN	198	48.749	1.145	19.915	1.00	45.12
ATOM	1089	C	GLN	198	48.585	2.547	20.514	1.00	44.49
ATOM	1090	O	GLN	198	49.435	3.400	20.303	1.00	47.79
ATOM	1084	CB	GLN	198	47.589	0.861	18.946	1.00	41.02
ATOM	1085	CG	GLN	198	47.516	-0.536	18.349	1.00	36.69
ATOM	1086	CD	GLN	198	46.274	-0.729	17.476	1.00	39.09
ATOM	1087	OE1	GLN	198	45.968	0.104	16.639	1.00	36.72
ATOM	1088	NE2	GLN	198	45.558	-1.828	17.677	1.00	39.10
ATOM	1091	N	TRP	199	47.554	2.778	21.326	1.00	44.54
ATOM	1092	CA	TRP	199	47.365	4.118	21.864	1.00	46.88
ATOM	1103	C	TRP	199	48.603	4.609	22.579	1.00	49.80
ATOM	1104	O	TRP	199	48.813	5.814	22.754	1.00	50.10
ATOM	1093	CB	TRP	199	46.060	4.262	22.682	1.00	49.31
ATOM	1094	CG	TRP	199	45.970	3.813	24.184	1.00	53.69
ATOM	1098	CD1	TRP	199	46.615	4.380	25.277	1.00	52.47
ATOM	1095	CD2	TRP	199	45.043	2.849	24.746	1.00	50.35
ATOM	1099	NE1	TRP	199	46.125	3.836	26.454	1.00	51.74
ATOM	1096	CE2	TRP	199	45.170	2.899	26.151	1.00	49.04
ATOM	1097	CE3	TRP	199	44.115	1.959	24.181	1.00	51.31
ATOM	1100	CZ2	TRP	199	44.412	2.089	26.998	1.00	53.08
ATOM	1101	CZ3	TRP	199	43.351	1.141	25.043	1.00	54.73
ATOM	1102	CH2	TRP	199	43.507	1.217	26.426	1.00	54.74
ATOM	1105	N	GLN	200	49.499	3.674	22.866	1.00	53.97
ATOM	1106	CA	GLN	200	50.752	4.023	23.522	1.00	58.62
ATOM	1112	C	GLN	200	51.801	4.474	22.495	1.00	60.14
ATOM	1113	O	GLN	200	53.001	4.560	22.776	1.00	60.70
ATOM	1107	CB	GLN	200	51.229	2.873	24.411	1.00	54.54
ATOM	1108	CG	GLN	200	50.383	2.755	25.678	1.00	54.36
ATOM	1109	CD	GLN	200	50.813	1.627	26.583	1.00	55.82
ATOM	1110	OE1	GLN	200	51.400	0.639	26.115	1.00	58.71
ATOM	1111	NE2	GLN	200	50.543	1.764	27.894	1.00	51.10
ATOM	1114	N	ARG	201	51.300	4.863	21.330	1.00	59.79
ATOM	1115	CA	ARG	201	52.131	5.328	20.244	1.00	61.29
ATOM	1117	C	ARG	201	51.393	6.433	19.490	1.00	63.96
ATOM	1118	O	ARG	201	51.915	6.960	18.494	1.00	66.88
ATOM	1116	CB	ARG	201	52.453	4.167	19.293	1.00	62.46
ATOM	1119	N	CYS	202	50.187	6.779	19.945	1.00	62.41
ATOM	1120	CA	CYS	202	49.391	7.832	19.303	1.00	63.40
ATOM	1123	C	CYS	202	48.563	8.507	20.384	1.00	64.22
ATOM	1124	O	CYS	202	47.829	7.835	21.131	1.00	66.32
ATOM	1121	CB	CYS	202	48.450	7.239	18.257	1.00	61.39
ATOM	1122	SG	CYS	202	49.270	6.169	17.020	1.00	79.62
ATOM	1125	N	GLY	203	48.662	9.830	20.468	1.00	63.17

Fig. 21V

ATOM	1126	CA	GLY	203	47.921	10.566	21.486	1.00	62.01
ATOM	1127	C	GLY	203	48.289	12.027	21.367	1.00	62.07
ATOM	1128	O	GLY	203	49.154	12.346	20.540	1.00	65.36
ATOM	1129	N	SER	204	47.679	12.877	22.195	1.00	61.18
ATOM	1130	CA	SER	204	47.888	14.332	22.192	1.00	62.35
ATOM	1133	C	SER	204	48.903	14.935	21.177	1.00	65.46
ATOM	1134	O	SER	204	48.651	14.827	19.936	1.00	68.87
ATOM	1131	CB	SER	204	48.165	14.832	23.613	1.00	59.85
ATOM	1132	OG	SER	204	47.912	16.230	23.680	1.00	61.90
ATOM	1139	N	ALA	209	55.720	19.006	13.772	1.00	54.11
ATOM	1140	CA	ALA	209	54.248	18.736	13.652	1.00	58.83
ATOM	1137	C	ALA	209	53.674	19.827	12.786	1.00	60.31
ATOM	1138	O	ALA	209	54.291	20.870	12.619	1.00	63.90
ATOM	1136	CB	ALA	209	53.542	18.737	15.006	1.00	59.22
ATOM	1141	N	SER	210	52.452	19.628	12.322	1.00	61.91
ATOM	1142	CA	SER	210	51.781	20.579	11.429	1.00	61.68
ATOM	1145	C	SER	210	50.896	21.633	12.162	1.00	60.77
ATOM	1146	O	SER	210	50.137	22.401	11.532	1.00	60.26
ATOM	1143	CB	SER	210	50.945	19.747	10.448	1.00	63.72
ATOM	1144	OG	SER	210	51.606	18.515	10.124	1.00	63.43
ATOM	1147	N	GLY	211	50.992	21.640	13.494	1.00	57.84
ATOM	1148	CA	GLY	211	50.217	22.561	14.297	1.00	55.55
ATOM	1149	C	GLY	211	48.778	22.100	14.486	1.00	54.23
ATOM	1150	O	GLY	211	48.498	20.907	14.517	1.00	55.02
ATOM	1151	N	ASP	212	47.863	23.050	14.630	1.00	50.53
ATOM	1152	CA	ASP	212	46.449	22.745	14.827	1.00	47.14
ATOM	1157	C	ASP	212	45.808	22.389	13.469	1.00	42.71
ATOM	1158	O	ASP	212	45.754	23.219	12.549	1.00	45.37
ATOM	1153	CB	ASP	212	45.759	23.954	15.478	1.00	45.05
ATOM	1154	CG	ASP	212	44.460	23.599	16.139	1.00	45.14
ATOM	1155	OD1	ASP	212	43.776	22.643	15.696	1.00	43.31
ATOM	1156	OD2	ASP	212	44.117	24.303	17.103	1.00	43.04
ATOM	1159	N	PRO	213	45.285	21.160	13.346	1.00	35.67
ATOM	1161	CA	PRO	213	44.661	20.700	12.109	1.00	31.78
ATOM	1164	C	PRO	213	43.277	21.259	11.818	1.00	32.46
ATOM	1165	O	PRO	213	42.731	21.048	10.724	1.00	36.10
ATOM	1162	CB	PRO	213	44.590	19.196	12.325	1.00	31.14
ATOM	1163	CG	PRO	213	44.346	19.081	13.808	1.00	30.49
ATOM	1160	CD	PRO	213	45.266	20.111	14.385	1.00	34.43
ATOM	1166	N	PHE	214	42.701	21.972	12.779	1.00	32.02
ATOM	1167	CA	PHE	214	41.338	22.476	12.622	1.00	28.90
ATOM	1175	C	PHE	214	41.279	23.760	11.873	1.00	27.51
ATOM	1176	O	PHE	214	41.722	24.780	12.368	1.00	27.26
ATOM	1168	CB	PHE	214	40.656	22.625	13.984	1.00	25.19
ATOM	1169	CG	PHE	214	39.175	22.917	13.912	1.00	18.12
ATOM	1170	CD1	PHE	214	38.278	21.935	13.516	1.00	13.31
ATOM	1171	CD2	PHE	214	38.677	24.172	14.304	1.00	18.16
ATOM	1172	CE1	PHE	214	36.907	22.189	13.515	1.00	13.17
ATOM	1173	CE2	PHE	214	37.291	24.439	14.304	1.00	16.89
ATOM	1174	CZ	PHE	214	36.411	23.439	13.911	1.00	13.74
ATOM	1177	N	ARG	215	40.634	23.723	10.721	1.00	29.52
ATOM	1178	CA	ARG	215	40.534	24.914	9.902	1.00	33.36
ATOM	1186	C	ARG	215	39.129	25.358	9.588	1.00	32.72
ATOM	1187	O	ARG	215	38.899	26.130	8.665	1.00	37.25

Fig. 21W

ATOM	1179	CB	ARG	215	41.384	24.757	8.643	1.00	34.33
ATOM	1180	CG	ARG	215	42.887	24.871	8.967	1.00	46.95
ATOM	1181	CD	ARG	215	43.771	24.409	7.843	1.00	53.60
ATOM	1182	NE	ARG	215	43.378	23.057	7.462	1.00	60.61
ATOM	1183	CZ	ARG	215	44.216	22.120	7.034	1.00	63.60
ATOM	1184	NH1	ARG	215	45.519	22.380	6.941	1.00	63.33
ATOM	1185	NH2	ARG	215	43.738	20.942	6.634	1.00	65.46
ATOM	1188	N	SER	216	38.170	24.830	10.319	1.00	30.58
ATOM	1189	CA	SER	216	36.788	25.247	10.128	1.00	27.44
ATOM	1192	C	SER	216	36.675	26.340	11.190	1.00	28.43
ATOM	1193	O	SER	216	37.695	26.884	11.654	1.00	25.95
ATOM	1190	CB	SER	216	35.824	24.093	10.435	1.00	26.03
ATOM	1191	OG	SER	216	34.455	24.469	10.369	1.00	31.02
ATOM	1194	N	ASP	217	35.453	26.597	11.640	1.00	30.09
ATOM	1195	CA	ASP	217	35.222	27.614	12.646	1.00	32.24
ATOM	1200	C	ASP	217	33.890	27.357	13.363	1.00	32.46
ATOM	1201	O	ASP	217	33.171	26.402	13.049	1.00	32.60
ATOM	1196	CB	ASP	217	35.248	29.036	12.012	1.00	29.83
ATOM	1197	CG	ASP	217	34.296	29.191	10.818	1.00	34.35
ATOM	1198	OD1	ASP	217	33.152	28.702	10.860	1.00	38.57
ATOM	1199	OD2	ASP	217	34.690	29.806	9.813	1.00	40.40
ATOM	1202	N	SER	218	33.530	28.306	14.218	1.00	30.22
ATOM	1203	CA	SER	218	32.311	28.271	14.996	1.00	28.39
ATOM	1206	C	SER	218	31.064	28.127	14.132	1.00	27.80
ATOM	1207	O	SER	218	30.148	27.366	14.463	1.00	25.20
ATOM	1204	CB	SER	218	32.227	29.562	15.799	1.00	28.12
ATOM	1205	OG	SER	218	31.321	29.381	16.855	1.00	32.39
ATOM	1208	N	TYR	219	31.053	28.853	13.018	1.00	25.85
ATOM	1209	CA	TYR	219	29.927	28.869	12.086	1.00	24.31
ATOM	1218	C	TYR	219	29.759	27.594	11.318	1.00	23.75
ATOM	1219	O	TYR	219	28.655	27.236	10.965	1.00	28.36
ATOM	1210	CB	TYR	219	30.079	30.003	11.100	1.00	25.49
ATOM	1211	CG	TYR	219	30.472	31.269	11.760	1.00	17.44
ATOM	1212	CD1	TYR	219	29.527	32.050	12.359	1.00	20.39
ATOM	1214	CD2	TYR	219	31.795	31.655	11.817	1.00	15.51
ATOM	1213	CE1	TYR	219	29.868	33.183	13.003	1.00	21.63
ATOM	1215	CE2	TYR	219	32.150	32.776	12.462	1.00	17.28
ATOM	1216	CZ	TYR	219	31.175	33.544	13.071	1.00	21.51
ATOM	1217	OH	TYR	219	31.503	34.633	13.851	1.00	25.64
ATOM	1220	N	GLY	220	30.844	26.900	11.058	1.00	21.69
ATOM	1221	CA	GLY	220	30.696	25.663	10.350	1.00	23.10
ATOM	1222	C	GLY	220	29.891	24.748	11.240	1.00	25.28
ATOM	1223	O	GLY	220	28.831	24.298	10.870	1.00	27.08
ATOM	1224	N	LEU	221	30.368	24.531	12.454	1.00	27.43
ATOM	1225	CA	LEU	221	29.687	23.663	13.400	1.00	23.85
ATOM	1230	C	LEU	221	28.232	24.050	13.574	1.00	24.86
ATOM	1231	O	LEU	221	27.379	23.188	13.646	1.00	28.26
ATOM	1226	CB	LEU	221	30.376	23.739	14.751	1.00	22.63
ATOM	1227	CG	LEU	221	31.629	22.918	15.039	1.00	23.32
ATOM	1228	CD1	LEU	221	31.930	21.947	13.929	1.00	16.81
ATOM	1229	CD2	LEU	221	32.786	23.839	15.343	1.00	25.13
ATOM	1232	N	LEU	222	27.942	25.338	13.703	1.00	24.44
ATOM	1233	CA	LEU	222	26.555	25.792	13.874	1.00	24.17
ATOM	1238	C	LEU	222	25.748	25.473	12.606	1.00	25.37

Fig. 21X

ATOM	1239	O	LEU	222	24.543	25.266	12.652	1.00	28.51
ATOM	1234	CB	LEU	222	26.530	27.294	14.158	1.00	18.10
ATOM	1235	CG	LEU	222	25.413	28.055	14.861	1.00	19.64
ATOM	1236	CD1	LEU	222	25.120	29.304	14.031	1.00	13.66
ATOM	1237	CD2	LEU	222	24.181	27.215	15.130	1.00	10.70
ATOM	1240	N	GLY	223	26.424	25.359	11.481	1.00	24.05
ATOM	1241	CA	GLY	223	25.716	25.084	10.260	1.00	23.57
ATOM	1242	C	GLY	223	25.230	23.673	10.187	1.00	24.92
ATOM	1243	O	GLY	223	24.158	23.435	9.644	1.00	27.83
ATOM	1244	N	ASN	224	26.024	22.721	10.668	1.00	26.40
ATOM	1245	CA	ASN	224	25.595	21.345	10.581	1.00	30.28
ATOM	1250	C	ASN	224	24.813	20.863	11.731	1.00	34.09
ATOM	1251	O	ASN	224	24.192	19.807	11.649	1.00	38.67
ATOM	1246	CB	ASN	224	26.680	20.343	10.150	1.00	37.71
ATOM	1247	CG	ASN	224	27.829	20.218	11.112	1.00	44.96
ATOM	1248	OD1	ASN	224	28.541	21.182	11.375	1.00	55.47
ATOM	1249	ND2	ASN	224	28.108	18.991	11.541	1.00	50.17
ATOM	1252	N	SER	225	24.703	21.710	12.750	1.00	37.86
ATOM	1253	CA	SER	225	23.920	21.378	13.938	1.00	36.97
ATOM	1256	C	SER	225	22.486	21.477	13.488	1.00	33.63
ATOM	1257	O	SER	225	21.629	20.885	14.132	1.00	39.97
ATOM	1254	CB	SER	225	24.125	22.387	15.059	1.00	39.46
ATOM	1255	OG	SER	225	23.501	23.624	14.706	1.00	45.03
ATOM	1258	N	VAL	226	22.221	22.300	12.459	1.00	27.68
ATOM	1259	CA	VAL	226	20.866	22.449	11.906	1.00	24.84
ATOM	1263	C	VAL	226	20.504	21.312	10.980	1.00	23.63
ATOM	1264	O	VAL	226	19.317	20.947	10.848	1.00	26.16
ATOM	1260	CB	VAL	226	20.650	23.752	11.146	1.00	26.42
ATOM	1261	CG1	VAL	226	19.152	23.936	10.845	1.00	27.11
ATOM	1262	CG2	VAL	226	21.122	24.897	11.997	1.00	34.71
ATOM	1265	N	ASP	227	21.503	20.778	10.296	1.00	19.92
ATOM	1266	CA	ASP	227	21.230	19.671	9.427	1.00	20.17
ATOM	1271	C	ASP	227	20.823	18.524	10.327	1.00	23.27
ATOM	1272	O	ASP	227	19.866	17.830	10.031	1.00	22.86
ATOM	1267	CB	ASP	227	22.466	19.254	8.669	1.00	22.84
ATOM	1268	CG	ASP	227	22.987	20.327	7.740	1.00	24.28
ATOM	1269	OD1	ASP	227	22.253	21.268	7.367	1.00	26.78
ATOM	1270	OD2	ASP	227	24.162	20.195	7.361	1.00	26.65
ATOM	1273	N	ALA	228	21.548	18.321	11.429	1.00	22.68
ATOM	1274	CA	ALA	228	21.238	17.214	12.331	1.00	22.37
ATOM	1276	C	ALA	228	19.809	17.262	12.792	1.00	25.35
ATOM	1277	O	ALA	228	19.206	16.231	13.044	1.00	28.84
ATOM	1275	CB	ALA	228	22.119	17.223	13.512	1.00	20.24
ATOM	1278	N	LEU	229	19.261	18.454	12.947	1.00	25.90
ATOM	1279	CA	LEU	229	17.875	18.578	13.377	1.00	23.79
ATOM	1284	C	LEU	229	16.930	17.923	12.351	1.00	25.05
ATOM	1285	O	LEU	229	15.775	17.617	12.648	1.00	29.62
ATOM	1280	CB	LEU	229	17.515	20.043	13.528	1.00	21.34
ATOM	1281	CG	LEU	229	17.565	20.861	14.813	1.00	27.66
ATOM	1282	CD1	LEU	229	18.840	20.742	15.550	1.00	32.14
ATOM	1283	CD2	LEU	229	17.411	22.307	14.376	1.00	28.67
ATOM	1286	N	TYR	230	17.415	17.675	11.152	1.00	24.44
ATOM	1287	CA	TYR	230	16.565	17.106	10.152	1.00	24.41
ATOM	1296	C	TYR	230	17.009	15.753	9.672	1.00	30.59

Fig. 21Y

ATOM	1297	O	TYR	230	16.853	15.417	8.490	1.00	34.38
ATOM	1288	CB	TYR	230	16.388	18.094	9.011	1.00	24.38
ATOM	1289	CG	TYR	230	15.606	19.291	9.453	1.00	22.41
ATOM	1290	CD1	TYR	230	16.212	20.301	10.199	1.00	23.91
ATOM	1292	CD2	TYR	230	14.224	19.363	9.227	1.00	18.72
ATOM	1291	CE1	TYR	230	15.438	21.372	10.746	1.00	24.68
ATOM	1293	CE2	TYR	230	13.462	20.403	9.753	1.00	24.11
ATOM	1294	CZ	TYR	230	14.072	21.397	10.522	1.00	23.61
ATOM	1295	OH	TYR	230	13.294	22.351	11.130	1.00	29.94
ATOM	1298	N	ILE	231	17.701	15.033	10.544	1.00	29.71
ATOM	1299	CA	ILE	231	18.066	13.672	10.234	1.00	31.94
ATOM	1304	C	ILE	231	16.915	12.951	10.960	1.00	37.44
ATOM	1305	O	ILE	231	16.638	13.218	12.141	1.00	35.38
ATOM	1300	CB	ILE	231	19.403	13.245	10.833	1.00	28.77
ATOM	1302	CG1	ILE	231	20.535	14.093	10.298	1.00	29.35
ATOM	1301	CG2	ILE	231	19.738	11.845	10.415	1.00	28.40
ATOM	1303	CD1	ILE	231	21.878	13.562	10.737	1.00	30.62
ATOM	1306	N	ARG	232	16.157	12.147	10.211	1.00	44.59
ATOM	1307	CA	ARG	232	15.030	11.415	10.779	1.00	44.65
ATOM	1308	C	ARG	232	15.458	10.198	11.573	1.00	44.35
ATOM	1309	O	ARG	232	16.465	9.559	11.284	1.00	44.03
ATOM	1310	N	GLU	233	14.681	9.854	12.584	1.00	44.58
ATOM	1311	CA	GLU	233	15.037	8.696	13.390	1.00	46.58
ATOM	1312	C	GLU	233	16.459	8.746	13.917	1.00	43.35
ATOM	1313	O	GLU	233	17.191	7.763	13.819	1.00	40.83
ATOM	1314	N	ARG	234	16.852	9.922	14.412	1.00	42.22
ATOM	1315	CA	ARG	234	18.181	10.123	14.978	1.00	39.03
ATOM	1323	C	ARG	234	18.149	9.484	16.353	1.00	36.42
ATOM	1324	O	ARG	234	18.690	8.411	16.521	1.00	38.06
ATOM	1316	CB	ARG	234	18.539	11.619	15.081	1.00	39.42
ATOM	1317	CG	ARG	234	20.014	11.958	15.441	1.00	35.93
ATOM	1318	CD	ARG	234	20.165	13.417	15.921	1.00	35.07
ATOM	1319	NE	ARG	234	21.500	13.705	16.481	1.00	46.22
ATOM	1320	CZ	ARG	234	21.884	13.494	17.752	1.00	42.40
ATOM	1321	NH1	ARG	234	21.056	12.956	18.635	1.00	40.75
ATOM	1322	NH2	ARG	234	23.114	13.804	18.140	1.00	35.29
ATOM	1325	N	LEU	235	17.428	10.068	17.304	1.00	35.64
ATOM	1326	CA	LEU	235	17.393	9.491	18.645	1.00	38.17
ATOM	1331	C	LEU	235	17.132	7.996	18.587	1.00	38.36
ATOM	1332	O	LEU	235	17.886	7.219	19.160	1.00	42.99
ATOM	1327	CB	LEU	235	16.391	10.201	19.559	1.00	41.07
ATOM	1328	CG	LEU	235	16.829	11.466	20.306	1.00	40.52
ATOM	1329	CD1	LEU	235	17.374	12.459	19.311	1.00	45.05
ATOM	1330	CD2	LEU	235	15.635	12.095	21.045	1.00	39.89
ATOM	1333	N	PRO	236	16.088	7.565	17.858	1.00	39.21
ATOM	1335	CA	PRO	236	15.796	6.130	17.753	1.00	37.61
ATOM	1338	C	PRO	236	17.026	5.302	17.324	1.00	33.37
ATOM	1339	O	PRO	236	17.377	4.318	17.958	1.00	34.59
ATOM	1336	CB	PRO	236	14.696	6.107	16.694	1.00	35.13
ATOM	1337	CG	PRO	236	13.902	7.316	17.078	1.00	35.05
ATOM	1334	CD	PRO	236	15.008	8.342	17.220	1.00	40.99
ATOM	1340	N	LYS	237	17.697	5.718	16.270	1.00	30.03
ATOM	1341	CA	LYS	237	18.844	4.989	15.844	1.00	28.46
ATOM	1347	C	LYS	237	19.896	4.996	16.952	1.00	29.82

Fig. 212

ATOM	1348	O	LYS	237	20.560	3.988	17.197	1.00	32.55
ATOM	1342	CB	LYS	237	19.403	5.613	14.588	1.00	26.78
ATOM	1343	CG	LYS	237	20.251	4.616	13.778	1.00	40.87
ATOM	1344	CD	LYS	237	21.781	4.899	13.724	1.00	36.29
ATOM	1345	CE	LYS	237	22.459	3.902	12.841	1.00	30.73
ATOM	1346	NZ	LYS	237	21.946	2.569	13.284	1.00	43.77
ATOM	1349	N	LEU	238	20.033	6.118	17.647	1.00	28.39
ATOM	1350	CA	LEU	238	21.037	6.217	18.690	1.00	28.54
ATOM	1355	C	LEU	238	20.697	5.370	19.899	1.00	31.28
ATOM	1356	O	LEU	238	21.589	4.778	20.534	1.00	33.98
ATOM	1351	CB	LEU	238	21.289	7.677	19.076	1.00	30.82
ATOM	1352	CG	LEU	238	22.233	8.539	18.208	1.00	27.93
ATOM	1353	CD1	LEU	238	22.006	9.987	18.605	1.00	26.37
ATOM	1354	CD2	LEU	238	23.718	8.133	18.350	1.00	20.29
ATOM	1357	N	ARG	239	19.409	5.255	20.195	1.00	29.28
ATOM	1358	CA	ARG	239	18.994	4.434	21.306	1.00	29.95
ATOM	1366	C	ARG	239	19.189	2.951	20.982	1.00	32.62
ATOM	1367	O	ARG	239	19.476	2.164	21.876	1.00	38.29
ATOM	1359	CB	ARG	239	17.564	4.748	21.693	1.00	33.28
ATOM	1360	CG	ARG	239	17.455	6.138	22.270	1.00	45.59
ATOM	1361	CD	ARG	239	16.230	6.334	23.133	1.00	50.39
ATOM	1362	NE	ARG	239	15.559	7.577	22.773	1.00	57.71
ATOM	1363	CZ	ARG	239	14.566	7.662	21.882	1.00	65.37
ATOM	1364	NH1	ARG	239	14.090	6.568	21.258	1.00	65.87
ATOM	1365	NH2	ARG	239	14.020	8.851	21.619	1.00	63.51
ATOM	1368	N	TYR	240	19.084	2.581	19.703	1.00	32.63
ATOM	1369	CA	TYR	240	19.256	1.204	19.230	1.00	31.79
ATOM	1378	C	TYR	240	20.719	0.807	19.325	1.00	30.50
ATOM	1379	O	TYR	240	21.052	-0.359	19.562	1.00	31.45
ATOM	1370	CB	TYR	240	18.788	1.113	17.769	1.00	35.95
ATOM	1371	CG	TYR	240	19.358	-0.053	16.982	1.00	38.78
ATOM	1372	CD1	TYR	240	20.653	-0.016	16.490	1.00	36.31
ATOM	1374	CD2	TYR	240	18.595	-1.204	16.738	1.00	42.29
ATOM	1373	CE1	TYR	240	21.179	-1.095	15.776	1.00	42.46
ATOM	1375	CE2	TYR	240	19.118	-2.302	16.011	1.00	37.93
ATOM	1376	CZ	TYR	240	20.409	-2.241	15.532	1.00	43.25
ATOM	1377	OH	TYR	240	20.938	-3.299	14.785	1.00	46.68
ATOM	1380	N	ASP	241	21.565	1.767	18.970	1.00	31.55
ATOM	1381	CA	ASP	241	23.022	1.659	19.014	1.00	31.08
ATOM	1386	C	ASP	241	23.595	1.432	20.430	1.00	32.84
ATOM	1387	O	ASP	241	24.339	0.471	20.651	1.00	33.81
ATOM	1382	CB	ASP	241	23.637	2.926	18.432	1.00	25.54
ATOM	1383	CG	ASP	241	23.556	2.981	16.936	1.00	26.72
ATOM	1384	OD1	ASP	241	23.377	1.938	16.280	1.00	29.52
ATOM	1385	OD2	ASP	241	23.703	4.083	16.393	1.00	28.20
ATOM	1388	N	LYS	242	23.280	2.309	21.382	1.00	30.91
ATOM	1389	CA	LYS	242	23.815	2.112	22.708	1.00	34.51
ATOM	1395	C	LYS	242	23.330	0.781	23.318	1.00	38.23
ATOM	1396	O	LYS	242	24.026	0.128	24.107	1.00	42.65
ATOM	1390	CB	LYS	242	23.508	3.316	23.606	1.00	34.78
ATOM	1391	CG	LYS	242	22.129	3.418	24.143	1.00	31.05
ATOM	1392	CD	LYS	242	22.094	4.487	25.164	1.00	35.26
ATOM	1393	CE	LYS	242	20.737	4.554	25.875	1.00	44.36
ATOM	1394	NZ	LYS	242	20.749	5.619	26.931	1.00	46.79

Fig. 21AA

ATOM	1397	N	GLN	243	22.154	0.347	22.903	1.00	40.07
ATOM	1398	CA	GLN	243	21.572	-0.915	23.372	1.00	43.12
ATOM	1404	C	GLN	243	22.263	-2.132	22.708	1.00	41.18
ATOM	1405	O	GLN	243	22.500	-3.157	23.356	1.00	42.71
ATOM	1399	CB	GLN	243	20.082	-0.875	23.055	1.00	46.95
ATOM	1400	CG	GLN	243	19.288	-2.114	23.250	1.00	52.35
ATOM	1401	CD	GLN	243	17.912	-1.939	22.608	1.00	63.31
ATOM	1402	OE1	GLN	243	17.715	-2.178	21.381	1.00	65.44
ATOM	1403	NE2	GLN	243	16.960	-1.447	23.408	1.00	63.81
ATOM	1406	N	LEU	244	22.608	-1.987	21.429	1.00	38.36
ATOM	1407	CA	LEU	244	23.284	-3.013	20.642	1.00	34.79
ATOM	1412	C	LEU	244	24.717	-3.231	21.163	1.00	38.42
ATOM	1413	O	LEU	244	25.131	-4.357	21.451	1.00	42.12
ATOM	1408	CB	LEU	244	23.318	-2.529	19.192	1.00	30.54
ATOM	1409	CG	LEU	244	23.842	-3.341	18.001	1.00	31.10
ATOM	1410	CD1	LEU	244	25.306	-3.078	17.734	1.00	25.64
ATOM	1411	CD2	LEU	244	23.555	-4.829	18.225	1.00	34.08
ATOM	1414	N	VAL	245	25.432	-2.116	21.335	1.00	37.64
ATOM	1415	CA	VAL	245	26.825	-2.017	21.786	1.00	30.53
ATOM	1419	C	VAL	245	27.036	-2.182	23.311	1.00	30.65
ATOM	1420	O	VAL	245	28.158	-2.400	23.783	1.00	28.44
ATOM	1416	CB	VAL	245	27.367	-0.681	21.240	1.00	29.97
ATOM	1417	CG1	VAL	245	28.068	0.101	22.296	1.00	30.95
ATOM	1418	CG2	VAL	245	28.229	-0.930	20.018	1.00	27.26
ATOM	1421	N	GLY	246	25.954	-2.037	24.080	1.00	32.34
ATOM	1422	CA	GLY	246	26.006	-2.252	25.521	1.00	31.25
ATOM	1423	C	GLY	246	26.468	-1.158	26.445	1.00	30.27
ATOM	1424	O	GLY	246	26.661	-1.403	27.622	1.00	32.71
ATOM	1425	N	VAL	247	26.627	0.044	25.923	1.00	29.11
ATOM	1426	CA	VAL	247	27.055	1.193	26.692	1.00	26.91
ATOM	1430	C	VAL	247	25.840	1.944	27.200	1.00	31.04
ATOM	1431	O	VAL	247	25.047	2.453	26.419	1.00	32.46
ATOM	1427	CB	VAL	247	27.859	2.099	25.824	1.00	24.79
ATOM	1428	CG1	VAL	247	28.121	3.418	26.529	1.00	24.35
ATOM	1429	CG2	VAL	247	29.135	1.385	25.458	1.00	22.52
ATOM	1432	N	THR	248	25.755	2.070	28.517	1.00	31.59
ATOM	1433	CA	THR	248	24.640	2.705	29.191	1.00	31.52
ATOM	1437	C	THR	248	24.940	4.096	29.706	1.00	30.82
ATOM	1438	O	THR	248	26.072	4.433	29.978	1.00	27.71
ATOM	1434	CB	THR	248	24.112	1.772	30.367	1.00	39.88
ATOM	1435	OG1	THR	248	25.123	1.511	31.381	1.00	37.28
ATOM	1436	CG2	THR	248	23.718	0.439	29.778	1.00	43.33
ATOM	1439	N	GLU	249	23.917	4.918	29.854	1.00	35.18
ATOM	1440	CA	GLU	249	24.137	6.260	30.375	1.00	40.09
ATOM	1446	C	GLU	249	24.388	6.151	31.862	1.00	40.92
ATOM	1447	O	GLU	249	24.469	7.158	32.542	1.00	44.71
ATOM	1441	CB	GLU	249	22.954	7.198	30.127	1.00	40.60
ATOM	1442	CG	GLU	249	21.724	6.826	30.887	1.00	50.58
ATOM	1443	CD	GLU	249	21.291	5.376	30.636	1.00	59.02
ATOM	1444	OE1	GLU	249	20.758	5.061	29.533	1.00	58.31
ATOM	1445	OE2	GLU	249	21.532	4.543	31.548	1.00	64.12
ATOM	1448	N	ARG	250	24.467	4.930	32.376	1.00	38.91
ATOM	1449	CA	ARG	250	24.739	4.747	33.786	1.00	40.07
ATOM	1457	C	ARG	250	26.252	4.528	34.031	1.00	38.25

Fig. 2188

ATOM	1458	O	ARG	250	26.748	4.725	35.146	1.00	32.79
ATOM	1450	CB	ARG	250	23.901	3.579	34.304	1.00	48.85
ATOM	1451	CG	ARG	250	23.800	3.482	35.806	1.00	51.71
ATOM	1452	CD	ARG	250	22.958	4.589	36.387	1.00	57.54
ATOM	1453	NE	ARG	250	23.239	4.740	37.813	1.00	60.92
ATOM	1454	CZ	ARG	250	24.274	5.427	38.313	1.00	64.84
ATOM	1455	NH1	ARG	250	25.136	6.081	37.503	1.00	62.54
ATOM	1456	NH2	ARG	250	24.428	5.489	39.639	1.00	61.35
ATOM	1459	N	GLU	251	26.975	4.215	32.950	1.00	37.29
ATOM	1460	CA	GLU	251	28.412	3.963	32.987	1.00	33.73
ATOM	1466	C	GLU	251	29.221	4.849	32.047	1.00	33.52
ATOM	1467	O	GLU	251	30.398	4.575	31.799	1.00	35.31
ATOM	1461	CB	GLU	251	28.720	2.495	32.653	1.00	35.71
ATOM	1462	CG	GLU	251	28.352	2.045	31.221	1.00	40.55
ATOM	1463	CD	GLU	251	29.442	1.178	30.544	1.00	43.48
ATOM	1464	OE1	GLU	251	30.384	0.720	31.240	1.00	42.46
ATOM	1465	OE2	GLU	251	29.351	0.957	29.313	1.00	38.78
ATOM	1468	N	SER	252	28.607	5.881	31.483	1.00	30.81
ATOM	1469	CA	SER	252	29.341	6.775	30.590	1.00	29.66
ATOM	1472	C	SER	252	28.526	8.036	30.411	1.00	25.67
ATOM	1473	O	SER	252	27.457	8.137	30.973	1.00	22.60
ATOM	1470	CB	SER	252	29.546	6.120	29.231	1.00	30.94
ATOM	1471	OG	SER	252	28.296	5.962	28.571	1.00	34.82
ATOM	1474	N	TYR	253	28.992	8.929	29.538	1.00	24.49
ATOM	1475	CA	TYR	253	28.334	10.202	29.238	1.00	22.09
ATOM	1484	C	TYR	253	27.370	10.233	28.055	1.00	20.73
ATOM	1485	O	TYR	253	27.037	11.301	27.572	1.00	21.44
ATOM	1476	CB	TYR	253	29.378	11.275	29.007	1.00	25.05
ATOM	1477	CG	TYR	253	30.250	11.528	30.192	1.00	21.90
ATOM	1478	CD1	TYR	253	31.421	10.822	30.377	1.00	25.70
ATOM	1480	CD2	TYR	253	29.911	12.489	31.111	1.00	24.11
ATOM	1479	CE1	TYR	253	32.221	11.069	31.432	1.00	25.12
ATOM	1481	CE2	TYR	253	30.694	12.746	32.168	1.00	22.43
ATOM	1482	CZ	TYR	253	31.839	12.039	32.327	1.00	25.62
ATOM	1483	OH	TYR	253	32.589	12.321	33.420	1.00	32.22
ATOM	1486	N	VAL	254	26.905	9.071	27.611	1.00	21.12
ATOM	1487	CA	VAL	254	25.960	8.932	26.496	1.00	20.15
ATOM	1491	C	VAL	254	24.739	9.786	26.768	1.00	23.00
ATOM	1492	O	VAL	254	24.074	9.622	27.776	1.00	28.92
ATOM	1488	CB	VAL	254	25.509	7.457	26.365	1.00	22.45
ATOM	1489	CG1	VAL	254	24.408	7.301	25.349	1.00	24.89
ATOM	1490	CG2	VAL	254	26.665	6.624	25.938	1.00	30.24
ATOM	1493	N	LYS	255	24.417	10.672	25.852	1.00	27.30
ATOM	1494	CA	LYS	255	23.275	11.538	26.022	1.00	30.38
ATOM	1500	C	LYS	255	22.063	10.999	25.260	1.00	35.51
ATOM	1501	O	LYS	255	20.934	11.434	25.474	1.00	40.15
ATOM	1495	CB	LYS	255	23.642	12.955	25.556	1.00	24.85
ATOM	1496	CG	LYS	255	24.794	13.563	26.334	1.00	23.95
ATOM	1497	CD	LYS	255	24.327	13.823	27.732	1.00	21.71
ATOM	1498	CE	LYS	255	25.409	14.193	28.711	1.00	23.83
ATOM	1499	NZ	LYS	255	24.792	14.656	30.029	1.00	28.73
ATOM	1502	N	ALA	256	22.291	10.044	24.379	1.00	39.90
ATOM	1503	CA	ALA	256	21.204	9.497	23.580	1.00	44.20
ATOM	1505	C	ALA	256	20.531	8.314	24.281	1.00	48.51

Fig. 21CC

ATOM	1506	O	ALA	256	21.207	7.279	24.465	1.00	51.64
ATOM	1504	CB	ALA	256	21.739	9.077	22.200	1.00	45.14
ATOM	1507	OXT	ALA	256	19.333	8.422	24.621	1.00	49.50
ATOM	1508	OH2	TIP	301	31.077	8.140	27.527	1.00	26.53
ATOM	1509	OH2	TIP	302	28.508	19.427	33.073	1.00	44.65
ATOM	1510	OH2	TIP	303	43.460	-2.890	5.012	1.00	47.04
ATOM	1511	OH2	TIP	304	34.353	1.990	5.346	1.00	60.54
ATOM	1512	OH2	TIP	305	40.811	-5.013	7.745	1.00	44.88
ATOM	1513	OH2	TIP	306	36.406	-9.018	7.810	1.00	45.38
ATOM	1514	OH2	TIP	307	42.194	-7.284	7.781	1.00	40.41
ATOM	1515	OH2	TIP	308	41.962	-3.068	10.961	1.00	43.60
ATOM	1516	OH2	TIP	309	32.124	-3.755	5.755	1.00	57.14
ATOM	1517	OH2	TIP	310	45.283	-4.742	8.388	1.00	66.05
ATOM	1518	OH2	TIP	311	42.408	1.268	2.187	1.00	48.23
ATOM	1519	OH2	TIP	312	33.724	-9.694	7.964	1.00	31.21
ATOM	1520	OH2	TIP	313	36.929	9.205	34.888	1.00	57.36
ATOM	1521	OH2	TIP	314	36.951	10.140	31.663	1.00	28.65
ATOM	1522	OH2	TIP	315	45.201	10.047	36.275	1.00	60.61
ATOM	1523	OH2	TIP	316	33.982	7.104	37.021	1.00	37.87
ATOM	1524	OH2	TIP	317	31.482	13.718	40.875	1.00	32.22
ATOM	1525	OH2	TIP	318	28.066	20.405	14.687	1.00	28.25
ATOM	1526	OH2	TIP	319	25.156	17.450	8.183	1.00	58.78
ATOM	1527	OH2	TIP	320	24.965	17.970	15.523	1.00	38.76
ATOM	1528	OH2	TIP	321	26.596	17.720	13.158	1.00	34.40
ATOM	1529	OH2	TIP	322	24.695	16.736	10.779	1.00	46.64
ATOM	1530	OH2	TIP	323	28.779	21.379	8.234	1.00	51.77
ATOM	1531	OH2	TIP	324	27.672	9.637	22.884	1.00	26.42
ATOM	1532	OH2	TIP	325	25.173	11.262	30.753	1.00	39.45
ATOM	1533	OH2	TIP	326	29.730	9.819	25.094	1.00	16.06
ATOM	1534	OH2	TIP	327	27.962	1.696	35.360	1.00	43.49
ATOM	1535	OH2	TIP	328	47.125	9.642	8.720	1.00	62.32
ATOM	1536	OH2	TIP	329	42.419	15.393	6.321	1.00	47.15
ATOM	1537	OH2	TIP	330	46.244	15.052	16.322	1.00	31.89
ATOM	1538	OH2	TIP	331	53.806	6.083	10.720	1.00	59.08
ATOM	1539	OH2	TIP	332	46.628	-11.519	15.104	1.00	59.71
ATOM	1540	OH2	TIP	333	44.954	19.739	26.592	1.00	59.39
ATOM	1541	OH2	TIP	334	12.217	15.492	8.254	1.00	49.78
ATOM	1542	OH2	TIP	335	33.333	28.433	7.372	1.00	41.13
ATOM	1543	OH2	TIP	336	31.448	3.643	9.698	1.00	27.38
ATOM	1544	OH2	TIP	337	32.521	7.362	2.579	1.00	61.89
ATOM	1545	OH2	TIP	338	13.938	-1.160	24.723	1.00	59.26
ATOM	1546	OH2	TIP	339	16.115	1.428	14.322	1.00	31.84
ATOM	1547	OH2	TIP	340	52.974	1.048	19.319	1.00	59.43
ATOM	1548	OH2	TIP	341	17.731	-0.160	26.396	1.00	59.51
ATOM	1549	OH2	TIP	342	25.870	6.267	15.266	1.00	28.55
ATOM	1550	OH2	TIP	343	35.943	-3.457	27.935	1.00	28.41
ATOM	1551	OH2	TIP	344	41.943	-11.451	27.321	1.00	48.13
ATOM	1552	OH2	TIP	345	42.449	20.182	4.040	1.00	45.54
ATOM	1553	OH2	TIP	346	38.786	9.933	-2.493	1.00	45.94
ATOM	1554	OH2	TIP	347	49.333	15.382	33.838	1.00	61.48
ATOM	1555	OH2	TIP	348	46.147	25.427	24.597	1.00	59.02
ATOM	1556	OH2	TIP	349	50.115	57.579	9.011	1.00	47.99
ATOM	1557	OH2	TIP	350	15.511	3.002	23.488	1.00	55.01
ATOM	1558	OH2	TIP	351	29.780	15.069	2.505	1.00	61.37

Fig. 21DD

ATOM	1559	OH2	TIP	352	31.338	-11.352	21.807	1.00	46.71
ATOM	1560	OH2	TIP	353	2.522	0.611	13.871	1.00	44.63
ATOM	1561	OH2	TIP	354	43.141	22.961	4.410	1.00	48.86
ATOM	1562	OH2	TIP	355	5.521	10.199	15.309	1.00	49.92
ATOM	1563	OH2	TIP	356	53.638	12.036	19.109	1.00	65.19
ATOM	1564	OH2	TIP	357	46.005	14.980	8.384	1.00	56.73
ATOM	1565	OH2	TIP	358	32.766	22.125	9.759	1.00	44.57
ATOM	1566	OH2	TIP	359	41.156	-11.512	31.108	1.00	59.78
ATOM	1567	OH2	TIP	360	54.373	1.466	7.933	1.00	64.65
ATOM	1568	OH2	TIP	361	-0.133	6.947	3.004	1.00	58.66
ATOM	1569	OH2	TIP	362	40.287	17.373	32.363	1.00	59.68
ATOM	1570	OH2	TIP	363	14.084	11.697	13.980	1.00	62.14
ATOM	1571	OH2	TIP	364	11.142	54.359	5.085	1.00	57.08
ATOM	1572	OH2	TIP	365	22.432	3.979	5.522	1.00	62.25
ATOM	1573	OH2	TIP	366	30.748	30.157	5.660	1.00	46.26
ATOM	1574	OH2	TIP	367	47.936	-6.613	17.774	1.00	62.86
ATOM	1575	OH2	TIP	368	33.450	31.881	8.631	1.00	62.94
ATOM	1576	OH2	TIP	369	50.764	2.321	11.268	1.00	48.17
ATOM	1577	OH2	TIP	370	45.493	3.077	13.078	1.00	56.73
ATOM	1578	OH2	TIP	371	38.224	-10.673	15.493	1.00	54.69
ATOM	1579	OH2	TIP	372	36.265	20.816	1.443	1.00	61.72
ATOM	1580	OH2	TIP	373	44.933	30.624	15.656	1.00	60.55

Fig. 22A

CRYST1	90.0	90.0	117.4	90.0	90.0	120.0	P6 ₄ 22
Residue							
Atom	AA	No	X	Y	Z	Occup'y	B Factor
ATOM 295	N	HIS 52	60.710	19.064	34.809	1.00	25.00
ATOM 296	CA	HIS 52	61.673	18.368	33.923	1.00	25.00
ATOM 297	C	HIS 52	62.853	19.281	33.567	1.00	25.00
ATOM 298	O	HIS 52	63.644	18.965	32.685	1.00	25.00
ATOM 299	CB	HIS 52	61.040	17.836	32.638	1.00	25.00
ATOM 300	CG	HIS 52	60.095	16.703	32.846	1.00	25.00
ATOM 301	ND1	HIS 52	60.477	15.394	33.018	1.00	25.00
ATOM 302	CD2	HIS 52	58.739	16.690	32.866	1.00	25.00
ATOM 304	CE1	HIS 52	59.365	14.648	33.133	1.00	25.00
ATOM 303	NE2	HIS 52	58.277	15.389	33.047	1.00	25.00
ATOM 316	N	LYS 54	66.220	20.501	33.661	1.00	25.00
ATOM 317	CA	LYS 54	67.571	20.028	33.907	1.00	25.00
ATOM 323	C	LYS 54	68.314	21.061	34.724	1.00	25.00
ATOM 324	O	LYS 54	69.184	20.710	35.497	1.00	25.00
ATOM 318	CB	LYS 54	68.306	19.831	32.566	1.00	25.00
ATOM 319	CG	LYS 54	67.562	18.902	31.571	1.00	25.00
ATOM 320	CD	LYS 54	68.311	18.646	30.254	1.00	25.00
ATOM 321	CE	LYS 54	67.565	17.600	29.383	1.00	25.00
ATOM 322	NZ	LYS 54	67.361	16.272	30.087	1.00	25.00
ATOM 833	N	SER 120	56.783	12.750	37.744	1.00	25.00
ATOM 834	CA	SER 120	56.871	12.264	36.371	1.00	25.00
ATOM 837	C	SER 120	58.207	11.615	36.106	1.00	25.00
ATOM 838	O	SER 120	59.223	12.257	36.207	1.00	25.00
ATOM 835	CB	SER 120	56.654	13.416	35.393	1.00	25.00
ATOM 836	OG	SER 120	55.882	13.005	34.260	1.00	25.00
ATOM 847	N	SER 122	60.685	10.577	33.743	1.00	25.00

Fig. 22B

Atom	Residue AA	No	X	Y	Z	Occup'y	B Factor
ATOM 848	CA	SER 122	61.107	10.697	32.356	1.00	25.00
ATOM 851	C	SER 122	62.017	9.485	32.133	1.00	25.00
ATOM 852	O	SER 122	63.223	9.520	32.442	1.00	25.00
ATOM 849	CB	SER 122	61.864	12.007	32.113	1.00	25.00
ATOM 850	OG	SER 122	61.773	12.871	33.244	1.00	25.00
ATOM 897	N	HIS 139	65.401	11.038	34.964	1.00	25.00
ATOM 898	CA	HIS 139	65.038	11.906	36.075	1.00	25.00
ATOM 899	C	HIS 139	63.544	11.855	36.391	1.00	25.00
ATOM 900	O	HIS 139	62.740	11.480	35.530	1.00	25.00
ATOM 901	CB	HIS 139	65.484	13.338	35.810	1.00	25.00
ATOM 902	CG	HIS 139	64.651	14.035	34.794	1.00	25.00
ATOM 903	ND1	HIS 139	63.791	15.068	35.084	1.00	25.00
ATOM 904	CD2	HIS 139	64.485	13.778	33.477	1.00	25.00
ATOM 906	CE1	HIS 139	63.141	15.388	33.977	1.00	25.00
ATOM 905	NE2	HIS 139	63.529	14.632	32.974	1.00	25.00
ATOM 927	N	CYS 143	55.349	17.841	39.601	1.00	25.00
ATOM 928	CA	CYS 143	54.419	18.608	38.783	1.00	25.00
ATOM 931	C	CYS 143	53.004	18.555	39.358	1.00	25.00
ATOM 932	O	CYS 143	52.801	17.928	40.375	1.00	25.00
ATOM 929	CB	CYS 143	54.426	17.953	37.403	1.00	25.00
ATOM 930	SG	CYS 143	54.272	16.114	37.477	1.00	25.00
ATOM 951	N	ARG 147	51.312	12.231	33.512	1.00	25.00
ATOM 952	CA	ARG 147	50.733	11.463	32.422	1.00	25.00
ATOM 960	C	ARG 147	50.256	10.082	32.917	1.00	25.00
ATOM 961	O	ARG 147	49.302	9.523	32.355	1.00	25.00
ATOM 953	CB	ARG 147	51.807	11.235	31.366	1.00	25.00
ATOM 954	CG	ARG 147	52.970	12.230	31.429	1.00	25.00
ATOM 955	CD	ARG 147	52.760	13.360	30.428	1.00	25.00

Fig. 22C

Atom	Residue		X	Y	Z	Occup'y	B Factor
	AA	No					
ATOM 956	NE	ARG 147	52.455	12.799	29.116	1.00	25.00
ATOM 957	CZ	ARG 147	53.210	11.894	28.492	1.00	25.00
ATOM 958	NH1	ARG 147	54.375	11.489	29.014	1.00	25.00
ATOM 959	NH2	ARG 147	52.815	11.430	27.314	1.00	25.00
ATOM 962	N	ARG 148	50.936	9.527	33.937	1.00	25.00
ATOM 963	CA	ARG 148	50.619	8.200	34.492	1.00	25.00
ATOM 971	C	ARG 148	49.540	8.123	35.562	1.00	25.00
ATOM 972	O	ARG 148	49.295	9.085	36.276	1.00	25.00
ATOM 964	CB	ARG 148	51.899	7.483	34.904	1.00	25.00
ATOM 965	CG	ARG 148	52.654	7.052	33.662	1.00	25.00
ATOM 966	CD	ARG 148	54.099	6.580	33.847	1.00	25.00
ATOM 967	NE	ARG 148	54.697	6.425	32.515	1.00	25.00
ATOM 968	CZ	ARG 148	55.985	6.252	32.253	1.00	25.00
ATOM 969	NH1	ARG 148	56.888	6.174	33.227	1.00	25.00
ATOM 970	NH2	ARG 148	56.356	6.145	30.987	1.00	25.00

Fig. 23A

CRYST1	89.990	89.990	117.420	90.00	90.00	120.00	P6422		
SCALE1	0.01111	0.00642	0.00000		0.00000				
SCALE2	0.00000	0.01283	0.00000		0.00000				
SCALE3	0.00000	0.00000	0.00852		0.00000				
ATOM	1	CB	GLU	11	64.652	21.405	57.653	1.00	25.00
ATOM	8	N	GLU	11	66.983	20.730	57.176	1.00	25.00
ATOM	9	CA	GLU	11	65.564	20.285	57.113	1.00	25.00
ATOM	6	C	GLU	11	65.166	19.833	55.677	1.00	25.00
ATOM	7	O	GLU	11	64.989	20.661	54.756	1.00	25.00
ATOM	1	CB	GLU	11	64.652	21.405	57.653	1.00	25.00
ATOM	2	CG	GLU	11	64.804	21.647	59.170	1.00	25.00
ATOM	3	CD	GLU	11	63.935	22.813	59.730	1.00	25.00
ATOM	4	OE1	GLU	11	63.962	23.921	59.115	1.00	25.00
ATOM	5	OE2	GLU	11	63.248	22.620	60.791	1.00	25.00
ATOM	10	N	ALA	12	65.051	18.518	55.488	1.00	25.00
ATOM	11	CA	ALA	12	64.697	17.975	54.179	1.00	25.00
ATOM	13	C	ALA	12	63.279	17.436	54.105	1.00	25.00
ATOM	14	O	ALA	12	62.554	17.388	55.088	1.00	25.00
ATOM	12	CB	ALA	12	65.686	16.883	53.766	1.00	25.00
ATOM	15	N	LEU	13	62.883	17.072	52.903	1.00	25.00
ATOM	16	CA	LEU	13	61.585	16.519	52.675	1.00	25.00
ATOM	21	C	LEU	13	61.864	15.223	51.980	1.00	25.00
ATOM	22	O	LEU	13	62.826	15.106	51.229	1.00	25.00
ATOM	17	CB	LEU	13	60.788	17.405	51.737	1.00	25.00
ATOM	18	CG	LEU	13	60.043	18.625	52.281	1.00	25.00
ATOM	19	CD1	LEU	13	61.000	19.515	53.084	1.00	25.00
ATOM	20	CD2	LEU	13	59.393	19.384	51.110	1.00	25.00
ATOM	23	N	TYR	14	61.065	14.223	52.290	1.00	25.00
ATOM	24	CA	TYR	14	61.202	12.941	51.658	1.00	25.00
ATOM	33	C	TYR	14	59.921	12.817	50.910	1.00	25.00
ATOM	34	O	TYR	14	58.871	13.223	51.408	1.00	25.00
ATOM	25	CB	TYR	14	61.322	11.846	52.697	1.00	25.00
ATOM	26	CG	TYR	14	62.613	11.952	53.420	1.00	25.00
ATOM	27	CD1	TYR	14	62.769	12.862	54.459	1.00	25.00

Fig. 23B

ATOM	29	CD2	TYR	14	63.730	11.254	52.973	1.00	25.00
ATOM	28	CE1	TYR	14	63.993	13.092	55.018	1.00	25.00
ATOM	30	CE2	TYR	14	64.975	11.480	53.535	1.00	25.00
ATOM	31	CZ	TYR	14	65.092	12.405	54.552	1.00	25.00
ATOM	32	OH	TYR	14	66.323	12.659	55.084	1.00	25.00
ATOM	35	N	VAL	15	60.030	12.353	49.676	1.00	25.00
ATOM	36	CA	VAL	15	58.886	12.157	48.807	1.00	25.00
ATOM	40	C	VAL	15	58.914	10.675	48.460	1.00	25.00
ATOM	41	O	VAL	15	59.998	10.114	48.276	1.00	25.00
ATOM	37	CB	VAL	15	59.064	12.948	47.511	1.00	25.00
ATOM	38	CG1	VAL	15	57.788	12.963	46.725	1.00	25.00
ATOM	39	CG2	VAL	15	59.519	14.337	47.809	1.00	25.00
ATOM	42	N	ALA	16	57.751	10.033	48.431	1.00	25.00
ATOM	43	CA	ALA	16	57.670	8.620	48.081	1.00	25.00
ATOM	45	C	ALA	16	56.377	8.391	47.299	1.00	25.00
ATOM	46	O	ALA	16	55.368	9.034	47.572	1.00	25.00
ATOM	44	CB	ALA	16	57.705	7.763	49.323	1.00	25.00
ATOM	47	N	GLY	17	56.417	7.527	46.291	1.00	25.00
ATOM	48	CA	GLY	17	55.240	7.254	45.489	1.00	25.00
ATOM	49	C	GLY	17	55.633	6.271	44.413	1.00	25.00
ATOM	50	O	GLY	17	56.784	5.847	44.365	1.00	25.00
ATOM	51	N	TYR	18	54.686	5.881	43.567	1.00	25.00
ATOM	52	CA	TYR	18	54.950	4.945	42.480	1.00	25.00
ATOM	61	C	TYR	18	55.305	5.694	41.223	1.00	25.00
ATOM	62	O	TYR	18	54.581	6.595	40.799	1.00	25.00
ATOM	53	CB	TYR	18	53.716	4.136	42.141	1.00	25.00
ATOM	54	CG	TYR	18	53.204	3.209	43.198	1.00	25.00
ATOM	55	CD1	TYR	18	53.712	1.935	43.317	1.00	25.00
ATOM	57	CD2	TYR	18	52.123	3.564	43.988	1.00	25.00
ATOM	56	CE1	TYR	18	53.170	1.043	44.163	1.00	25.00
ATOM	58	CE2	TYR	18	51.573	2.675	44.842	1.00	25.00
ATOM	59	CZ	TYR	18	52.099	1.408	44.922	1.00	25.00
ATOM	60	OH	TYR	18	51.517	0.472	45.743	1.00	25.00
ATOM	63	N	LEU	19	56.378	5.278	40.578	1.00	25.00
ATOM	64	CA	LEU	19	56.784	5.927	39.344	1.00	25.00
ATOM	69	C	LEU	19	55.732	5.619	38.284	1.00	25.00
ATOM	70	O	LEU	19	55.461	6.452	37.413	1.00	25.00

Fig. 23C

ATOM	65	CB	LEU	19	58.146	5.392	38.897	1.00	25.00
ATOM	66	CG	LEU	19	59.417	6.149	39.272	1.00	25.00
ATOM	67	CD1	LEU	19	59.159	7.068	40.422	1.00	25.00
ATOM	68	CD2	LEU	19	60.550	5.181	39.574	1.00	25.00
ATOM	71	N	ALA	20	55.131	4.429	38.381	1.00	25.00
ATOM	72	CA	ALA	20	54.120	3.967	37.420	1.00	25.00
ATOM	74	C	ALA	20	53.390	2.696	37.880	1.00	25.00
ATOM	75	O	ALA	20	53.970	1.838	38.565	1.00	25.00
ATOM	73	CB	ALA	20	54.787	3.694	36.073	1.00	25.00
ATOM	76	N	LEU	21	52.118	2.565	37.518	1.00	25.00
ATOM	77	CA	LEU	21	51.403	1.361	37.903	1.00	25.00
ATOM	82	C	LEU	21	51.393	0.435	36.707	1.00	25.00
ATOM	83	O	LEU	21	51.003	0.847	35.601	1.00	25.00
ATOM	78	CB	LEU	21	49.984	1.659	38.388	1.00	25.00
ATOM	79	CG	LEU	21	49.814	2.274	39.784	1.00	25.00
ATOM	80	CD1	LEU	21	48.358	2.185	40.179	1.00	25.00
ATOM	81	CD2	LEU	21	50.660	1.548	40.796	1.00	25.00
ATOM	84	N	TYR	22	51.863	-0.796	36.927	1.00	25.00
ATOM	85	CA	TYR	22	51.955	-1.816	35.880	1.00	25.00
ATOM	94	C	TYR	22	50.657	-1.941	35.107	1.00	25.00
ATOM	95	O	TYR	22	49.583	-2.239	35.687	1.00	25.00
ATOM	86	CB	TYR	22	52.384	-3.173	36.445	1.00	25.00
ATOM	87	CG	TYR	22	53.827	-3.230	36.948	1.00	25.00
ATOM	88	CD1	TYR	22	54.827	-2.416	36.416	1.00	25.00
ATOM	90	CD2	TYR	22	54.188	-4.112	37.961	1.00	25.00
ATOM	89	CE1	TYR	22	56.141	-2.496	36.892	1.00	25.00
ATOM	91	CE2	TYR	22	55.490	-4.189	38.433	1.00	25.00
ATOM	92	CZ	TYR	22	56.451	-3.387	37.903	1.00	25.00
ATOM	93	OH	TYR	22	57.708	-3.482	38.422	1.00	25.00
ATOM	96	N	SER	23	50.773	-1.593	33.816	1.00	25.00
ATOM	97	CA	SER	23	49.653	-1.616	32.887	1.00	25.00
ATOM	98	C	SER	23	48.792	-0.355	32.875	1.00	25.00
ATOM	99	O	SER	23	48.745	0.376	31.883	1.00	25.00
ATOM	100	N	LYS	24	48.143	-0.088	34.001	1.00	25.00
ATOM	101	CA	LYS	24	47.243	1.054	34.177	1.00	25.00
ATOM	103	C	LYS	24	47.583	2.417	33.503	1.00	25.00
ATOM	104	O	LYS	24	46.681	3.073	32.914	1.00	25.00

Fig. 23D

ATOM	102	CB	LYS	24	46.959	1.244	35.672	1.00	25.00
ATOM	105	N	ASP	25	48.853	2.844	33.590	1.00	25.00
ATOM	106	CA	ASP	25	49.292	4.112	32.993	1.00	25.00
ATOM	111	C	ASP	25	48.991	4.227	31.492	1.00	25.00
ATOM	112	O	ASP	25	48.985	5.340	30.964	1.00	25.00
ATOM	107	CB	ASP	25	50.775	4.346	33.244	1.00	25.00
ATOM	108	CG	ASP	25	51.659	3.274	32.623	1.00	25.00
ATOM	109	OD1	ASP	25	51.148	2.256	32.088	1.00	25.00
ATOM	110	OD2	ASP	25	52.898	3.450	32.697	1.00	25.00
ATOM	113	N	GLU	26	48.773	3.080	30.823	1.00	25.00
ATOM	114	CA	GLU	26	48.431	2.985	29.384	1.00	25.00
ATOM	116	C	GLU	26	49.606	2.876	28.430	1.00	25.00
ATOM	117	O	GLU	26	50.760	2.879	28.852	1.00	25.00
ATOM	115	CB	GLU	26	47.516	4.146	28.946	1.00	25.00
ATOM	118	N	GLY	27	49.288	2.753	27.142	1.00	25.00
ATOM	119	CA	GLY	27	50.301	2.640	26.098	1.00	25.00
ATOM	120	C	GLY	27	51.475	3.615	26.150	1.00	25.00
ATOM	121	O	GLY	27	51.401	4.653	26.828	1.00	25.00
ATOM	122	N	GLU	28	52.533	3.295	25.392	1.00	25.00
ATOM	123	CA	GLU	28	53.771	4.087	25.351	1.00	25.00
ATOM	129	C	GLU	28	54.317	4.289	26.767	1.00	25.00
ATOM	130	O	GLU	28	55.269	3.619	27.176	1.00	25.00
ATOM	124	CB	GLU	28	53.557	5.444	24.673	1.00	25.00
ATOM	125	CG	GLU	28	53.502	5.391	23.144	1.00	25.00
ATOM	126	CD	GLU	28	52.088	5.556	22.585	1.00	25.00
ATOM	127	OE1	GLU	28	51.226	4.655	22.848	1.00	25.00
ATOM	128	OE2	GLU	28	51.861	6.582	21.874	1.00	25.00
ATOM	131	N	LEU	29	53.669	5.187	27.509	1.00	25.00
ATOM	132	CA	LEU	29	53.999	5.497	28.892	1.00	25.00
ATOM	137	C	LEU	29	54.172	4.218	29.684	1.00	25.00
ATOM	138	O	LEU	29	54.892	4.204	30.685	1.00	25.00
ATOM	133	CB	LEU	29	52.848	6.255	29.544	1.00	25.00
ATOM	134	CG	LEU	29	52.537	7.687	29.124	1.00	25.00
ATOM	135	CD1	LEU	29	53.753	8.537	29.390	1.00	25.00
ATOM	136	CD2	LEU	29	52.112	7.765	27.662	1.00	25.00
ATOM	139	N	ASN	30	53.446	3.172	29.277	1.00	25.00
ATOM	140	CA	ASN	30	53.476	1.883	29.955	1.00	25.00

Fig. 23E

ATOM	145	C	ASN	30	54.845	1.368	30.373	1.00	25.00
ATOM	146	O	ASN	30	55.776	1.317	29.575	1.00	25.00
ATOM	141	CB	ASN	30	52.728	0.810	29.155	1.00	25.00
ATOM	142	CG	ASN	30	51.554	0.202	29.953	1.00	25.00
ATOM	143	OD1	ASN	30	51.752	-0.393	31.028	1.00	25.00
ATOM	144	ND2	ASN	30	50.329	0.364	29.439	1.00	25.00
ATOM	147	N	ILE	31	54.961	1.033	31.656	1.00	25.00
ATOM	148	CA	ILE	31	56.187	0.494	32.242	1.00	25.00
ATOM	153	C	ILE	31	55.901	-0.976	32.612	1.00	25.00
ATOM	154	O	ILE	31	54.780	-1.327	33.010	1.00	25.00
ATOM	149	CB	ILE	31	56.610	1.339	33.473	1.00	25.00
ATOM	151	CG1	ILE	31	57.091	2.719	33.006	1.00	25.00
ATOM	150	CG2	ILE	31	57.701	0.638	34.247	1.00	25.00
ATOM	152	CD1	ILE	31	58.052	2.649	31.817	1.00	25.00
ATOM	155	N	THR	32	56.881	-1.851	32.445	1.00	25.00
ATOM	156	CA	THR	32	56.638	-3.256	32.731	1.00	25.00
ATOM	160	C	THR	32	57.860	-3.886	33.383	1.00	25.00
ATOM	161	O	THR	32	58.980	-3.347	33.261	1.00	25.00
ATOM	157	CB	THR	32	56.320	-4.018	31.431	1.00	25.00
ATOM	158	OG1	THR	32	57.539	-4.216	30.694	1.00	25.00
ATOM	159	CG2	THR	32	55.310	-3.224	30.549	1.00	25.00
ATOM	162	N	PRO	33	57.682	-5.064	34.034	1.00	25.00
ATOM	164	CA	PRO	33	58.763	-5.794	34.722	1.00	25.00
ATOM	167	C	PRO	33	60.101	-6.010	33.954	1.00	25.00
ATOM	168	O	PRO	33	61.182	-5.770	34.515	1.00	25.00
ATOM	165	CB	PRO	33	58.069	-7.093	35.157	1.00	25.00
ATOM	166	CG	PRO	33	56.674	-6.634	35.446	1.00	25.00
ATOM	163	CD	PRO	33	56.392	-5.749	34.236	1.00	25.00
ATOM	169	N	GLU	34	60.039	-6.437	32.688	1.00	25.00
ATOM	170	CA	GLU	34	61.245	-6.634	31.857	1.00	25.00
ATOM	176	C	GLU	34	62.063	-5.346	31.882	1.00	25.00
ATOM	177	O	GLU	34	63.288	-5.364	31.766	1.00	25.00
ATOM	171	CB	GLU	34	60.836	-6.927	30.395	1.00	25.00
ATOM	172	CG	GLU	34	62.000	-7.209	29.377	1.00	25.00
ATOM	173	CD	GLU	34	61.689	-8.375	28.350	1.00	25.00
ATOM	174	OE1	GLU	34	60.516	-8.524	27.873	1.00	25.00
ATOM	175	OE2	GLU	34	62.639	-9.144	28.024	1.00	25.00

Fig. 23F

ATOM	178	N	ILE	35	61.353	-4.238	32.072	1.00	25.00
ATOM	179	CA	ILE	35	61.931	-2.910	32.093	1.00	25.00
ATOM	184	C	ILE	35	62.427	-2.524	33.464	1.00	25.00
ATOM	185	O	ILE	35	63.538	-2.027	33.623	1.00	25.00
ATOM	180	CB	ILE	35	60.886	-1.877	31.637	1.00	25.00
ATOM	182	CG1	ILE	35	60.131	-2.417	30.415	1.00	25.00
ATOM	181	CG2	ILE	35	61.566	-0.567	31.293	1.00	25.00
ATOM	183	CD1	ILE	35	59.063	-1.500	29.855	1.00	25.00
ATOM	186	N	VAL	36	61.584	-2.739	34.457	1.00	25.00
ATOM	187	CA	VAL	36	61.930	-2.391	35.831	1.00	25.00
ATOM	191	C	VAL	36	63.210	-3.095	36.263	1.00	25.00
ATOM	192	O	VAL	36	64.262	-2.475	36.453	1.00	25.00
ATOM	188	CB	VAL	36	60.824	-2.826	36.807	1.00	25.00
ATOM	189	CG1	VAL	36	60.849	-1.952	38.030	1.00	25.00
ATOM	190	CG2	VAL	36	59.483	-2.787	36.142	1.00	25.00
ATOM	193	N	ARG	37	63.085	-4.414	36.390	1.00	25.00
ATOM	194	CA	ARG	37	64.162	-5.309	36.818	1.00	25.00
ATOM	196	C	ARG	37	65.469	-5.054	36.065	1.00	25.00
ATOM	197	O	ARG	37	66.567	-5.111	36.650	1.00	25.00
ATOM	195	CB	ARG	37	63.716	-6.779	36.669	1.00	25.00
ATOM	198	N	SER	38	65.358	-4.820	34.763	1.00	25.00
ATOM	199	CA	SER	38	66.551	-4.526	34.001	1.00	25.00
ATOM	202	C	SER	38	67.092	-3.191	34.532	1.00	25.00
ATOM	203	O	SER	38	68.214	-3.130	35.026	1.00	25.00
ATOM	200	CB	SER	38	66.244	-4.464	32.478	1.00	25.00
ATOM	201	OG	SER	38	65.138	-3.623	32.113	1.00	25.00
ATOM	204	N	ALA	39	66.219	-2.184	34.551	1.00	25.00
ATOM	205	CA	ALA	39	66.525	-0.821	34.977	1.00	25.00
ATOM	207	C	ALA	39	67.130	-0.599	36.392	1.00	25.00
ATOM	208	O	ALA	39	67.855	0.386	36.637	1.00	25.00
ATOM	206	CB	ALA	39	65.280	0.036	34.794	1.00	25.00
ATOM	209	N	LEU	40	66.815	-1.470	37.341	1.00	25.00
ATOM	210	CA	LEU	40	67.358	-1.284	38.690	1.00	25.00
ATOM	215	C	LEU	40	68.290	-2.446	39.056	1.00	25.00
ATOM	216	O	LEU	40	68.205	-3.530	38.472	1.00	25.00
ATOM	211	CB	LEU	40	66.226	-1.127	39.722	1.00	25.00
ATOM	212	CG	LEU	40	64.816	-0.832	39.178	1.00	25.00

Fig. 23G

ATOM	213	CD1	LEU	40	63.823	-0.837	40.308	1.00	25.00
ATOM	214	CD2	LEU	40	64.774	0.493	38.422	1.00	25.00
ATOM	217	N	PRO	41	69.259	-2.205	39.949	1.00	25.00
ATOM	219	CA	PRO	41	69.482	-0.910	40.587	1.00	25.00
ATOM	222	C	PRO	41	70.020	-0.005	39.485	1.00	25.00
ATOM	223	O	PRO	41	70.869	-0.435	38.684	1.00	25.00
ATOM	220	CB	PRO	41	70.590	-1.210	41.617	1.00	25.00
ATOM	221	CG	PRO	41	70.747	-2.770	41.632	1.00	25.00
ATOM	218	CD	PRO	41	70.375	-3.130	40.225	1.00	25.00
ATOM	224	N	PRO	42	69.476	1.223	39.371	1.00	25.00
ATOM	226	CA	PRO	42	69.891	2.217	38.351	1.00	25.00
ATOM	229	C	PRO	42	71.379	2.556	38.489	1.00	25.00
ATOM	230	O	PRO	42	71.867	2.756	39.615	1.00	25.00
ATOM	227	CB	PRO	42	69.016	3.435	38.675	1.00	25.00
ATOM	228	CG	PRO	42	67.755	2.795	39.308	1.00	25.00
ATOM	225	CD	PRO	42	68.369	1.731	40.211	1.00	25.00
ATOM	231	N	THR	43	72.100	2.618	37.366	1.00	25.00
ATOM	232	CA	THR	43	73.534	2.908	37.450	1.00	25.00
ATOM	236	C	THR	43	73.772	4.334	37.932	1.00	25.00
ATOM	237	O	THR	43	74.441	4.566	38.944	1.00	25.00
ATOM	233	CB	THR	43	74.297	2.675	36.097	1.00	25.00
ATOM	234	OG1	THR	43	74.154	3.822	35.237	1.00	25.00
ATOM	235	CG2	THR	43	73.770	1.406	35.379	1.00	25.00
ATOM	238	N	SER	44	73.158	5.280	37.234	1.00	25.00
ATOM	239	CA	SER	44	73.315	6.690	37.557	1.00	25.00
ATOM	241	C	SER	44	72.327	7.201	38.592	1.00	25.00
ATOM	242	O	SER	44	71.103	7.118	38.401	1.00	25.00
ATOM	240	CB	SER	44	73.229	7.531	36.278	1.00	25.00
ATOM	243	N	LYS	45	72.878	7.741	39.676	1.00	25.00
ATOM	244	CA	LYS	45	72.093	8.305	40.764	1.00	25.00
ATOM	246	C	LYS	45	71.058	9.285	40.193	1.00	25.00
ATOM	247	O	LYS	45	71.386	10.415	39.834	1.00	25.00
ATOM	245	CB	LYS	45	73.006	9.005	41.736	1.00	25.00
ATOM	248	N	ILE	46	69.818	8.809	40.113	1.00	25.00
ATOM	249	CA	ILE	46	68.681	9.534	39.567	1.00	25.00
ATOM	254	C	ILE	46	68.292	10.768	40.340	1.00	25.00
ATOM	255	O	ILE	46	68.077	10.703	41.549	1.00	25.00

Fig. 23H

ATOM	250	CB	ILE	46	67.480	8.617	39.497	1.00	25.00
ATOM	252	CG1	ILE	46	67.832	7.407	38.646	1.00	25.00
ATOM	251	CG2	ILE	46	66.304	9.335	38.902	1.00	25.00
ATOM	253	CD1	ILE	46	66.677	6.468	38.460	1.00	25.00
ATOM	256	N	PRO	47	68.167	11.907	39.642	1.00	25.00
ATOM	258	CA	PRO	47	67.803	13.197	40.219	1.00	25.00
ATOM	261	C	PRO	47	66.334	13.605	40.104	1.00	25.00
ATOM	262	O	PRO	47	65.599	13.164	39.223	1.00	25.00
ATOM	259	CB	PRO	47	68.708	14.152	39.461	1.00	25.00
ATOM	260	CG	PRO	47	68.638	13.600	38.081	1.00	25.00
ATOM	257	CD	PRO	47	68.722	12.090	38.288	1.00	25.00
ATOM	263	N	ILE	48	65.950	14.511	40.990	1.00	25.00
ATOM	264	CA	ILE	48	64.603	15.035	41.070	1.00	25.00
ATOM	269	C	ILE	48	64.613	16.526	40.742	1.00	25.00
ATOM	270	O	ILE	48	65.226	17.328	41.436	1.00	25.00
ATOM	265	CB	ILE	48	64.024	14.778	42.499	1.00	25.00
ATOM	267	CG1	ILE	48	63.421	13.385	42.564	1.00	25.00
ATOM	266	CG2	ILE	48	62.999	15.822	42.911	1.00	25.00
ATOM	268	CD1	ILE	48	62.725	13.102	43.855	1.00	25.00
ATOM	271	N	ASN	49	63.997	16.897	39.640	1.00	25.00
ATOM	272	CA	ASN	49	63.940	18.302	39.306	1.00	25.00
ATOM	277	C	ASN	49	62.477	18.674	39.152	1.00	25.00
ATOM	278	O	ASN	49	61.608	17.807	39.219	1.00	25.00
ATOM	273	CB	ASN	49	64.791	18.643	38.064	1.00	25.00
ATOM	274	CG	ASN	49	64.249	18.060	36.775	1.00	25.00
ATOM	275	OD1	ASN	49	63.041	17.877	36.617	1.00	25.00
ATOM	276	ND2	ASN	49	65.147	17.795	35.822	1.00	25.00
ATOM	279	N	ILE	50	62.205	19.952	38.949	1.00	25.00
ATOM	280	CA	ILE	50	60.845	20.456	38.816	1.00	25.00
ATOM	285	C	ILE	50	60.554	20.807	37.355	1.00	25.00
ATOM	286	O	ILE	50	61.366	21.443	36.727	1.00	25.00
ATOM	281	CB	ILE	50	60.707	21.745	39.670	1.00	25.00
ATOM	283	CG1	ILE	50	60.974	21.459	41.145	1.00	25.00
ATOM	282	CG2	ILE	50	59.367	22.430	39.417	1.00	25.00
ATOM	284	CD1	ILE	50	61.054	22.697	41.962	1.00	25.00
ATOM	287	N	ASP	51	59.416	20.383	36.817	1.00	25.00
ATOM	288	CA	ASP	51	59.018	20.705	35.437	1.00	25.00

Fig. 23I

ATOM	293	C	ASP	51	59.915	20.048	34.386	1.00	25.00
ATOM	294	O	ASP	51	59.833	20.381	33.194	1.00	25.00
ATOM	289	CB	ASP	51	59.010	22.251	35.251	1.00	25.00
ATOM	290	CG	ASP	51	58.470	22.728	33.852	1.00	25.00
ATOM	291	OD1	ASP	51	57.376	22.260	33.453	1.00	25.00
ATOM	292	OD2	ASP	51	59.111	23.607	33.183	1.00	25.00
ATOM	295	N	HIS	52	60.710	19.064	34.809	1.00	25.00
ATOM	296	CA	HIS	52	61.673	18.368	33.923	1.00	25.00
ATOM	297	C	HIS	52	62.853	19.281	33.567	1.00	25.00
ATOM	298	O	HIS	52	63.644	18.965	32.685	1.00	25.00
ATOM	299	CB	HIS	52	61.040	17.836	32.638	1.00	25.00
ATOM	300	CG	HIS	52	60.095	16.703	32.846	1.00	25.00
ATOM	301	ND1	HIS	52	60.477	15.394	33.018	1.00	25.00
ATOM	302	CD2	HIS	52	58.739	16.690	32.866	1.00	25.00
ATOM	304	CE1	HIS	52	59.365	14.648	33.133	1.00	25.00
ATOM	303	NE2	HIS	52	58.277	15.389	33.047	1.00	25.00
ATOM	305	N	ARG	53	62.972	20.396	34.290	1.00	25.00
ATOM	306	CA	ARG	53	64.033	21.369	34.117	1.00	25.00
ATOM	314	C	ARG	53	65.376	20.861	34.610	1.00	25.00
ATOM	315	O	ARG	53	65.645	20.811	35.799	1.00	25.00
ATOM	307	CB	ARG	53	63.690	22.672	34.839	1.00	25.00
ATOM	308	CG	ARG	53	62.664	23.523	34.126	1.00	25.00
ATOM	309	CD	ARG	53	63.218	24.057	32.816	1.00	25.00
ATOM	310	NE	ARG	53	63.931	25.325	32.972	1.00	25.00
ATOM	311	CZ	ARG	53	63.342	26.522	32.907	1.00	25.00
ATOM	312	NH1	ARG	53	62.022	26.597	32.679	1.00	25.00
ATOM	313	NH2	ARG	53	64.063	27.643	33.061	1.00	25.00
ATOM	316	N	LYS	54	66.220	20.501	33.661	1.00	25.00
ATOM	317	CA	LYS	54	67.571	20.028	33.907	1.00	25.00
ATOM	323	C	LYS	54	68.314	21.061	34.724	1.00	25.00
ATOM	324	O	LYS	54	69.184	20.710	35.497	1.00	25.00
ATOM	318	CB	LYS	54	68.306	19.831	32.566	1.00	25.00
ATOM	319	CG	LYS	54	67.562	18.902	31.571	1.00	25.00
ATOM	320	CD	LYS	54	68.311	18.646	30.254	1.00	25.00
ATOM	321	CE	LYS	54	67.565	17.600	29.383	1.00	25.00
ATOM	322	NZ	LYS	54	67.361	16.272	30.087	1.00	25.00
ATOM	325	N	ASP	55	67.979	22.334	34.535	1.00	25.00

Fig. 23J

ATOM	326	CA	ASP	55	68.618	23.436	35.261	1.00	25.00
ATOM	331	C	ASP	55	67.939	23.679	36.575	1.00	25.00
ATOM	332	O	ASP	55	68.259	24.648	37.267	1.00	25.00
ATOM	327	CB	ASP	55	68.567	24.746	34.464	1.00	25.00
ATOM	328	CG	ASP	55	67.144	25.164	34.100	1.00	25.00
ATOM	329	OD1	ASP	55	66.229	24.318	34.100	1.00	25.00
ATOM	330	OD2	ASP	55	66.934	26.353	33.792	1.00	25.00
ATOM	333	N	CYS	56	66.952	22.846	36.887	1.00	25.00
ATOM	334	CA	CYS	56	66.214	23.006	38.127	1.00	25.00
ATOM	337	C	CYS	56	66.002	21.704	38.893	1.00	25.00
ATOM	338	O	CYS	56	64.889	21.210	38.989	1.00	25.00
ATOM	335	CB	CYS	56	64.885	23.704	37.864	1.00	25.00
ATOM	336	SG	CYS	56	64.114	24.218	39.393	1.00	25.00
ATOM	339	N	VAL	57	67.099	21.153	39.410	1.00	25.00
ATOM	340	CA	VAL	57	67.127	19.908	40.182	1.00	25.00
ATOM	344	C	VAL	57	67.134	20.364	41.619	1.00	25.00
ATOM	345	O	VAL	57	67.836	21.312	41.955	1.00	25.00
ATOM	341	CB	VAL	57	68.410	19.098	39.887	1.00	25.00
ATOM	342	CG1	VAL	57	68.506	17.900	40.795	1.00	25.00
ATOM	343	CG2	VAL	57	68.437	18.662	38.420	1.00	25.00
ATOM	346	N	VAL	58	66.359	19.686	42.459	1.00	25.00
ATOM	347	CA	VAL	58	66.219	20.055	43.870	1.00	25.00
ATOM	351	C	VAL	58	66.341	18.905	44.868	1.00	25.00
ATOM	352	O	VAL	58	65.980	19.065	46.042	1.00	25.00
ATOM	348	CB	VAL	58	64.844	20.705	44.116	1.00	25.00
ATOM	349	CG1	VAL	58	64.765	22.056	43.428	1.00	25.00
ATOM	350	CG2	VAL	58	63.745	19.782	43.605	1.00	25.00
ATOM	353	N	GLY	59	66.833	17.759	44.416	1.00	25.00
ATOM	354	CA	GLY	59	66.963	16.622	45.298	1.00	25.00
ATOM	355	C	GLY	59	67.369	15.450	44.449	1.00	25.00
ATOM	356	O	GLY	59	67.750	15.646	43.286	1.00	25.00
ATOM	357	N	GLU	60	67.322	14.243	45.012	1.00	25.00
ATOM	358	CA	GLU	60	67.686	13.036	44.271	1.00	25.00
ATOM	364	C	GLU	60	67.033	11.777	44.843	1.00	25.00
ATOM	365	O	GLU	60	66.983	11.592	46.072	1.00	25.00
ATOM	359	CB	GLU	60	69.212	12.848	44.234	1.00	25.00
ATOM	360	CG	GLU	60	69.852	12.284	45.524	1.00	25.00

Fig. 23K

ATOM	361	CD	GLU	60	71.256	11.712	45.294	1.00	25.00
ATOM	362	OE1	GLU	60	71.446	10.930	44.343	1.00	25.00
ATOM	363	OE2	GLU	60	72.171	12.048	46.065	1.00	25.00
ATOM	366	N	VAL	61	66.508	10.935	43.952	1.00	25.00
ATOM	367	CA	VAL	61	65.886	9.659	44.329	1.00	25.00
ATOM	371	C	VAL	61	66.937	8.836	45.099	1.00	25.00
ATOM	372	O	VAL	61	67.976	8.487	44.538	1.00	25.00
ATOM	368	CB	VAL	61	65.451	8.852	43.047	1.00	25.00
ATOM	369	CG1	VAL	61	65.395	7.351	43.321	1.00	25.00
ATOM	370	CG2	VAL	61	64.097	9.317	42.566	1.00	25.00
ATOM	373	N	ILE	62	66.679	8.529	46.367	1.00	25.00
ATOM	374	CA	ILE	62	67.647	7.750	47.123	1.00	25.00
ATOM	379	C	ILE	62	67.451	6.248	46.991	1.00	25.00
ATOM	380	O	ILE	62	68.322	5.497	47.396	1.00	25.00
ATOM	375	CB	ILE	62	67.737	8.168	48.624	1.00	25.00
ATOM	377	CG1	ILE	62	66.593	7.592	49.433	1.00	25.00
ATOM	376	CG2	ILE	62	67.738	9.688	48.762	1.00	25.00
ATOM	378	CD1	ILE	62	66.488	8.209	50.816	1.00	25.00
ATOM	381	N	ALA	63	66.334	5.817	46.398	1.00	25.00
ATOM	382	CA	ALA	63	66.037	4.388	46.207	1.00	25.00
ATOM	384	C	ALA	63	64.724	4.115	45.473	1.00	25.00
ATOM	385	O	ALA	63	63.744	4.831	45.649	1.00	25.00
ATOM	383	CB	ALA	63	66.020	3.660	47.549	1.00	25.00
ATOM	386	N	ILE	64	64.712	3.042	44.685	1.00	25.00
ATOM	387	CA	ILE	64	63.537	2.613	43.905	1.00	25.00
ATOM	392	C	ILE	64	63.441	1.080	43.999	1.00	25.00
ATOM	393	O	ILE	64	64.432	0.390	43.766	1.00	25.00
ATOM	388	CB	ILE	64	63.676	2.934	42.362	1.00	25.00
ATOM	390	CG1	ILE	64	64.256	4.330	42.118	1.00	25.00
ATOM	389	CG2	ILE	64	62.313	2.841	41.680	1.00	25.00
ATOM	391	CD1	ILE	64	64.319	4.721	40.652	1.00	25.00
ATOM	394	N	ILE	65	62.294	0.540	44.391	1.00	25.00
ATOM	395	CA	ILE	65	62.182	-0.899	44.440	1.00	25.00
ATOM	400	C	ILE	65	61.117	-1.269	43.481	1.00	25.00
ATOM	401	O	ILE	65	60.446	-0.413	42.908	1.00	25.00
ATOM	396	CB	ILE	65	61.750	-1.452	45.788	1.00	25.00
ATOM	398	CG1	ILE	65	60.384	-0.896	46.189	1.00	25.00

Fig. 23L

ATOM	397	CG2	ILE	65	62.819	-1.200	46.825	1.00	25.00
ATOM	399	CD1	ILE	65	59.638	-1.796	47.154	1.00	25.00
ATOM	402	N	GLU	66	60.885	-2.564	43.395	1.00	25.00
ATOM	403	CA	GLU	66	59.882	-3.089	42.500	1.00	25.00
ATOM	409	C	GLU	66	58.789	-3.706	43.336	1.00	25.00
ATOM	410	O	GLU	66	59.044	-4.669	44.064	1.00	25.00
ATOM	404	CB	GLU	66	60.512	-4.151	41.625	1.00	25.00
ATOM	405	CG	GLU	66	59.561	-4.789	40.693	1.00	25.00
ATOM	406	CD	GLU	66	60.152	-6.023	40.097	1.00	25.00
ATOM	407	OE1	GLU	66	61.365	-6.003	39.750	1.00	25.00
ATOM	408	OE2	GLU	66	59.397	-7.023	40.000	1.00	25.00
ATOM	411	N	ASP	67	57.607	-3.096	43.291	1.00	25.00
ATOM	412	CA	ASP	67	56.445	-3.571	44.039	1.00	25.00
ATOM	417	C	ASP	67	55.530	-4.430	43.162	1.00	25.00
ATOM	418	O	ASP	67	55.565	-4.351	41.928	1.00	25.00
ATOM	413	CB	ASP	67	55.665	-2.388	44.633	1.00	25.00
ATOM	414	CG	ASP	67	54.319	-2.801	45.221	1.00	25.00
ATOM	415	OD1	ASP	67	54.250	-3.859	45.876	1.00	25.00
ATOM	416	OD2	ASP	67	53.321	-2.069	45.034	1.00	25.00
ATOM	419	N	ILE	68	54.741	-5.283	43.812	1.00	25.00
ATOM	420	CA	ILE	68	53.792	-6.155	43.131	1.00	25.00
ATOM	425	C	ILE	68	52.962	-5.288	42.155	1.00	25.00
ATOM	426	O	ILE	68	52.624	-5.724	41.056	1.00	25.00
ATOM	421	CB	ILE	68	52.880	-6.877	44.197	1.00	25.00
ATOM	423	CG1	ILE	68	52.891	-8.387	43.996	1.00	25.00
ATOM	422	CG2	ILE	68	51.445	-6.397	44.117	1.00	25.00
ATOM	424	CD1	ILE	68	52.313	-8.821	42.685	1.00	25.00
ATOM	427	N	ARG	69	52.698	-4.044	42.572	1.00	25.00
ATOM	428	CA	ARG	69	51.919	-3.072	41.808	1.00	25.00
ATOM	436	C	ARG	69	52.718	-2.195	40.859	1.00	25.00
ATOM	437	O	ARG	69	52.160	-1.698	39.900	1.00	25.00
ATOM	429	CB	ARG	69	51.124	-2.158	42.751	1.00	25.00
ATOM	430	CG	ARG	69	49.915	-2.788	43.450	1.00	25.00
ATOM	431	CD	ARG	69	49.025	-1.716	44.155	1.00	25.00
ATOM	432	NE	ARG	69	48.399	-0.768	43.222	1.00	25.00
ATOM	433	CZ	ARG	69	47.253	-0.118	43.427	1.00	25.00
ATOM	434	NH1	ARG	69	46.514	-0.293	44.525	1.00	25.00

Fig. 23M

ATOM	435	NH2	ARG	69	46.826	0.703	42.493	1.00	25.00
ATOM	438	N	GLY	70	53.983	-1.936	41.167	1.00	25.00
ATOM	439	CA	GLY	70	54.798	-1.095	40.298	1.00	25.00
ATOM	440	C	GLY	70	56.075	-0.545	40.920	1.00	25.00
ATOM	441	O	GLY	70	56.417	-0.918	42.026	1.00	25.00
ATOM	442	N	PRO	71	56.843	0.289	40.215	1.00	25.00
ATOM	444	CA	PRO	71	58.057	0.809	40.836	1.00	25.00
ATOM	447	C	PRO	71	57.633	1.785	41.929	1.00	25.00
ATOM	448	O	PRO	71	56.783	2.649	41.669	1.00	25.00
ATOM	445	CB	PRO	71	58.719	1.582	39.689	1.00	25.00
ATOM	446	CG	PRO	71	58.175	0.965	38.472	1.00	25.00
ATOM	443	CD	PRO	71	56.746	0.743	38.824	1.00	25.00
ATOM	449	N	PHE	72	58.213	1.655	43.128	1.00	25.00
ATOM	450	CA	PHE	72	57.923	2.548	44.263	1.00	25.00
ATOM	458	C	PHE	72	59.233	3.224	44.646	1.00	25.00
ATOM	459	O	PHE	72	60.240	2.545	44.823	1.00	25.00
ATOM	451	CB	PHE	72	57.368	1.764	45.450	1.00	25.00
ATOM	452	CG	PHE	72	56.866	2.633	46.561	1.00	25.00
ATOM	453	CD1	PHE	72	55.580	3.151	46.527	1.00	25.00
ATOM	454	CD2	PHE	72	57.688	2.970	47.624	1.00	25.00
ATOM	455	CE1	PHE	72	55.125	3.998	47.536	1.00	25.00
ATOM	456	CE2	PHE	72	57.239	3.814	48.631	1.00	25.00
ATOM	457	CZ	PHE	72	55.961	4.329	48.586	1.00	25.00
ATOM	460	N	PHE	73	59.233	4.546	44.774	1.00	25.00
ATOM	461	CA	PHE	73	60.467	5.252	45.080	1.00	25.00
ATOM	469	C	PHE	73	60.412	6.130	46.277	1.00	25.00
ATOM	470	O	PHE	73	59.354	6.517	46.733	1.00	25.00
ATOM	462	CB	PHE	73	60.912	6.118	43.898	1.00	25.00
ATOM	463	CG	PHE	73	60.369	7.551	43.913	1.00	25.00
ATOM	464	CD1	PHE	73	59.016	7.816	43.726	1.00	25.00
ATOM	465	CD2	PHE	73	61.228	8.626	44.052	1.00	25.00
ATOM	466	CE1	PHE	73	58.544	9.114	43.674	1.00	25.00
ATOM	467	CE2	PHE	73	60.753	9.918	44.001	1.00	25.00
ATOM	468	CZ	PHE	73	59.414	10.160	43.812	1.00	25.00
ATOM	471	N	LEU	74	61.588	6.528	46.714	1.00	25.00
ATOM	472	CA	LEU	74	61.739	7.413	47.851	1.00	25.00
ATOM	477	C	LEU	74	62.815	8.398	47.396	1.00	25.00

Fig. 23N

ATOM	478	O	LEU	74	63.735	8.034	46.663	1.00	25.00
ATOM	473	CB	LEU	74	62.170	6.608	49.086	1.00	25.00
ATOM	474	CG	LEU	74	62.373	7.314	50.429	1.00	25.00
ATOM	475	CD1	LEU	74	61.160	8.119	50.809	1.00	25.00
ATOM	476	CD2	LEU	74	62.639	6.270	51.483	1.00	25.00
ATOM	479	N	GLY	75	62.675	9.656	47.744	1.00	25.00
ATOM	480	CA	GLY	75	63.681	10.579	47.301	1.00	25.00
ATOM	481	C	GLY	75	63.844	11.660	48.324	1.00	25.00
ATOM	482	O	GLY	75	63.045	11.771	49.265	1.00	25.00
ATOM	483	N	ILE	76	64.914	12.425	48.178	1.00	25.00
ATOM	484	CA	ILE	76	65.150	13.518	49.087	1.00	25.00
ATOM	489	C	ILE	76	65.138	14.855	48.317	1.00	25.00
ATOM	490	O	ILE	76	65.635	14.954	47.183	1.00	25.00
ATOM	485	CB	ILE	76	66.440	13.292	49.933	1.00	25.00
ATOM	487	CG1	ILE	76	66.501	14.288	51.084	1.00	25.00
ATOM	486	CG2	ILE	76	67.687	13.406	49.090	1.00	25.00
ATOM	488	CD1	ILE	76	67.476	13.896	52.139	1.00	25.00
ATOM	491	N	VAL	77	64.407	15.817	48.875	1.00	25.00
ATOM	492	CA	VAL	77	64.291	17.156	48.319	1.00	25.00
ATOM	496	C	VAL	77	64.801	18.074	49.435	1.00	25.00
ATOM	497	O	VAL	77	64.118	18.362	50.418	1.00	25.00
ATOM	493	CB	VAL	77	62.818	17.482	47.865	1.00	25.00
ATOM	494	CG1	VAL	77	62.675	18.941	47.430	1.00	25.00
ATOM	495	CG2	VAL	77	62.417	16.561	46.715	1.00	25.00
ATOM	498	N	ARG	78	66.075	18.404	49.326	1.00	25.00
ATOM	499	CA	ARG	78	66.745	19.263	50.277	1.00	25.00
ATOM	507	C	ARG	78	67.311	20.433	49.464	1.00	25.00
ATOM	508	O	ARG	78	68.421	20.352	48.940	1.00	25.00
ATOM	500	CB	ARG	78	67.866	18.473	50.959	1.00	25.00
ATOM	501	CG	ARG	78	68.655	19.225	52.024	1.00	25.00
ATOM	502	CD	ARG	78	69.818	18.351	52.511	1.00	25.00
ATOM	503	NE	ARG	78	69.379	17.274	53.393	1.00	25.00
ATOM	504	CZ	ARG	78	69.600	17.263	54.710	1.00	25.00
ATOM	505	NH1	ARG	78	70.350	18.222	55.267	1.00	25.00
ATOM	506	NH2	ARG	78	69.135	16.255	55.466	1.00	25.00
ATOM	509	N	CYS	79	66.495	21.473	49.285	1.00	25.00
ATOM	510	CA	CYS	79	66.873	22.682	48.537	1.00	25.00

Fig. 230

ATOM	513	C	CYS	79	66.384	23.872	49.360	1.00	25.00
ATOM	514	O	CYS	79	65.192	24.121	49.475	1.00	25.00
ATOM	511	CB	CYS	79	66.240	22.689	47.122	1.00	25.00
ATOM	512	SG	CYS	79	66.357	24.292	46.237	1.00	25.00
ATOM	515	N	PRO	80	67.300	24.608	49.978	1.00	25.00
ATOM	517	CA	PRO	80	66.819	25.737	50.769	1.00	25.00
ATOM	520	C	PRO	80	66.026	26.759	49.987	1.00	25.00
ATOM	521	O	PRO	80	65.062	27.306	50.513	1.00	25.00
ATOM	518	CB	PRO	80	68.103	26.328	51.363	1.00	25.00
ATOM	519	CG	PRO	80	69.142	26.002	50.341	1.00	25.00
ATOM	516	CD	PRO	80	68.769	24.559	49.954	1.00	25.00
ATOM	522	N	GLN	81	66.374	26.987	48.728	1.00	25.00
ATOM	523	CA	GLN	81	65.643	27.985	47.953	1.00	25.00
ATOM	529	C	GLN	81	64.189	27.601	47.656	1.00	25.00
ATOM	530	O	GLN	81	63.296	28.455	47.693	1.00	25.00
ATOM	524	CB	GLN	81	66.386	28.340	46.661	1.00	25.00
ATOM	525	CG	GLN	81	67.700	29.107	46.868	1.00	25.00
ATOM	526	CD	GLN	81	68.774	28.254	47.500	1.00	25.00
ATOM	527	OE1	GLN	81	68.818	27.045	47.284	1.00	25.00
ATOM	528	NE2	GLN	81	69.619	28.863	48.315	1.00	25.00
ATOM	531	N	LEU	82	63.947	26.311	47.420	1.00	25.00
ATOM	532	CA	LEU	82	62.604	25.827	47.124	1.00	25.00
ATOM	537	C	LEU	82	61.583	26.245	48.168	1.00	25.00
ATOM	538	O	LEU	82	60.447	26.505	47.820	1.00	25.00
ATOM	533	CB	LEU	82	62.611	24.317	46.944	1.00	25.00
ATOM	534	CG	LEU	82	61.407	23.536	46.406	1.00	25.00
ATOM	535	CD1	LEU	82	60.679	22.850	47.550	1.00	25.00
ATOM	536	CD2	LEU	82	60.489	24.397	45.571	1.00	25.00
ATOM	539	N	HIS	83	61.979	26.340	49.438	1.00	25.00
ATOM	540	CA	HIS	83	61.049	26.759	50.496	1.00	25.00
ATOM	547	C	HIS	83	60.968	28.279	50.590	1.00	25.00
ATOM	548	O	HIS	83	59.910	28.839	50.890	1.00	25.00
ATOM	541	CB	HIS	83	61.462	26.249	51.868	1.00	25.00
ATOM	542	CG	HIS	83	61.604	24.767	51.960	1.00	25.00
ATOM	544	ND1	HIS	83	61.658	24.106	53.171	1.00	25.00
ATOM	543	CD2	HIS	83	61.806	23.826	51.006	1.00	25.00
ATOM	545	CE1	HIS	83	61.902	22.824	52.960	1.00	25.00

Fig. 23P

ATOM	546	NE2	HIS	83	61.996	22.629	51.656	1.00	25.00
ATOM	549	N	ALA	84	62.087	28.948	50.367	1.00	25.00
ATOM	550	CA	ALA	84	62.104	30.389	50.465	1.00	25.00
ATOM	552	C	ALA	84	61.208	31.109	49.465	1.00	25.00
ATOM	553	O	ALA	84	60.433	31.966	49.873	1.00	25.00
ATOM	551	CB	ALA	84	63.512	30.897	50.369	1.00	25.00
ATOM	554	N	VAL	85	61.271	30.734	48.180	1.00	25.00
ATOM	555	CA	VAL	85	60.472	31.395	47.121	1.00	25.00
ATOM	559	C	VAL	85	58.948	31.205	47.241	1.00	25.00
ATOM	560	O	VAL	85	58.165	32.113	46.923	1.00	25.00
ATOM	556	CB	VAL	85	60.980	31.063	45.634	1.00	25.00
ATOM	557	CG1	VAL	85	62.370	30.462	45.645	1.00	25.00
ATOM	558	CG2	VAL	85	59.987	30.186	44.857	1.00	25.00
ATOM	561	N	LEU	86	58.563	30.021	47.709	1.00	25.00
ATOM	562	CA	LEU	86	57.184	29.623	47.921	1.00	25.00
ATOM	567	C	LEU	86	56.663	30.418	49.116	1.00	25.00
ATOM	568	O	LEU	86	55.654	31.094	49.034	1.00	25.00
ATOM	563	CB	LEU	86	57.163	28.117	48.197	1.00	25.00
ATOM	564	CG	LEU	86	56.290	27.177	47.365	1.00	25.00
ATOM	565	CD1	LEU	86	56.116	27.695	45.983	1.00	25.00
ATOM	566	CD2	LEU	86	56.901	25.791	47.331	1.00	25.00
ATOM	569	N	PHE	87	57.389	30.370	50.221	1.00	25.00
ATOM	570	CA	PHE	87	57.016	31.105	51.422	1.00	25.00
ATOM	578	C	PHE	87	56.751	32.579	51.089	1.00	25.00
ATOM	579	O	PHE	87	55.846	33.221	51.633	1.00	25.00
ATOM	571	CB	PHE	87	58.149	31.014	52.435	1.00	25.00
ATOM	572	CG	PHE	87	58.007	29.895	53.414	1.00	25.00
ATOM	573	CD1	PHE	87	56.793	29.244	53.584	1.00	25.00
ATOM	574	CD2	PHE	87	59.084	29.523	54.206	1.00	25.00
ATOM	575	CE1	PHE	87	56.656	28.240	54.531	1.00	25.00
ATOM	576	CE2	PHE	87	58.958	28.529	55.150	1.00	25.00
ATOM	577	CZ	PHE	87	57.743	27.883	55.318	1.00	25.00
ATOM	580	N	GLU	88	57.603	33.121	50.235	1.00	25.00
ATOM	581	CA	GLU	88	57.476	34.481	49.803	1.00	25.00
ATOM	587	C	GLU	88	56.176	34.597	49.040	1.00	25.00
ATOM	588	O	GLU	88	55.391	35.470	49.343	1.00	25.00
ATOM	582	CB	GLU	88	58.636	34.818	48.901	1.00	25.00

Fig. 23Q

ATOM	583	CG	GLU	88	58.746	36.262	48.501	1.00	25.00
ATOM	584	CD	GLU	88	60.010	36.527	47.667	1.00	25.00
ATOM	585	OE1	GLU	88	60.333	35.691	46.767	1.00	25.00
ATOM	586	OE2	GLU	88	60.678	37.566	47.922	1.00	25.00
ATOM	589	N	ALA	89	55.918	33.686	48.094	1.00	25.00
ATOM	590	CA	ALA	89	54.686	33.705	47.253	1.00	25.00
ATOM	592	C	ALA	89	53.341	33.663	48.002	1.00	25.00
ATOM	593	O	ALA	89	52.361	34.303	47.578	1.00	25.00
ATOM	591	CB	ALA	89	54.723	32.574	46.188	1.00	25.00
ATOM	594	N	ALA	90	53.288	32.875	49.077	1.00	25.00
ATOM	595	CA	ALA	90	52.082	32.741	49.874	1.00	25.00
ATOM	597	C	ALA	90	51.714	34.106	50.464	1.00	25.00
ATOM	598	O	ALA	90	52.585	34.880	50.855	1.00	25.00
ATOM	596	CB	ALA	90	52.309	31.741	50.954	1.00	25.00
ATOM	599	N	HIS	91	50.426	34.420	50.496	1.00	25.00
ATOM	600	CA	HIS	91	49.969	35.703	51.021	1.00	25.00
ATOM	607	C	HIS	91	50.205	35.729	52.517	1.00	25.00
ATOM	608	O	HIS	91	50.284	34.665	53.161	1.00	25.00
ATOM	601	CB	HIS	91	48.459	35.881	50.798	1.00	25.00
ATOM	602	CG	HIS	91	48.078	36.359	49.431	1.00	25.00
ATOM	604	ND1	HIS	91	46.794	36.245	48.939	1.00	25.00
ATOM	603	CD2	HIS	91	48.794	36.987	48.468	1.00	25.00
ATOM	605	CE1	HIS	91	46.736	36.785	47.734	1.00	25.00
ATOM	606	NE2	HIS	91	47.938	37.241	47.425	1.00	25.00
ATOM	609	N	SER	92	50.182	36.943	53.077	1.00	25.00
ATOM	610	CA	SER	92	50.343	37.154	54.527	1.00	25.00
ATOM	613	C	SER	92	49.399	36.278	55.373	1.00	25.00
ATOM	614	O	SER	92	49.573	36.172	56.597	1.00	25.00
ATOM	611	CB	SER	92	50.090	38.630	54.906	1.00	25.00
ATOM	612	OG	SER	92	51.302	39.368	55.070	1.00	25.00
ATOM	615	N	ASN	93	48.366	35.710	54.755	1.00	25.00
ATOM	616	CA	ASN	93	47.474	34.879	55.525	1.00	25.00
ATOM	621	C	ASN	93	47.243	33.446	55.082	1.00	25.00
ATOM	622	O	ASN	93	46.230	32.799	55.400	1.00	25.00
ATOM	617	CB	ASN	93	46.211	35.633	55.871	1.00	25.00
ATOM	618	CG	ASN	93	46.481	36.729	56.875	1.00	25.00
ATOM	619	OD1	ASN	93	47.000	37.803	56.512	1.00	25.00

Fig. 23R

ATOM	620	ND2	ASN	93	46.227	36.438	58.161	1.00	25.00
ATOM	623	N	PHE	94	48.187	32.938	54.314	1.00	25.00
ATOM	624	CA	PHE	94	48.094	31.549	53.968	1.00	25.00
ATOM	632	C	PHE	94	48.509	31.036	55.358	1.00	25.00
ATOM	633	O	PHE	94	49.521	31.493	55.918	1.00	25.00
ATOM	625	CB	PHE	94	49.138	31.202	52.903	1.00	25.00
ATOM	626	CG	PHE	94	48.881	29.899	52.223	1.00	25.00
ATOM	627	CD1	PHE	94	49.285	28.710	52.809	1.00	25.00
ATOM	628	CD2	PHE	94	48.173	29.856	51.030	1.00	25.00
ATOM	629	CE1	PHE	94	48.984	27.506	52.226	1.00	25.00
ATOM	630	CE2	PHE	94	47.868	28.656	50.440	1.00	25.00
ATOM	631	CZ	PHE	94	48.273	27.473	51.039	1.00	25.00
ATOM	634	N	PHE	95	47.677	30.203	55.962	1.00	25.00
ATOM	635	CA	PHE	95	47.939	29.658	57.307	1.00	25.00
ATOM	643	C	PHE	95	47.372	30.641	58.317	1.00	25.00
ATOM	644	O	PHE	95	47.767	31.802	58.335	1.00	25.00
ATOM	636	CB	PHE	95	49.438	29.469	57.631	1.00	25.00
ATOM	637	CG	PHE	95	50.154	28.502	56.734	1.00	25.00
ATOM	638	CD1	PHE	95	49.797	27.167	56.699	1.00	25.00
ATOM	639	CD2	PHE	95	51.191	28.932	55.919	1.00	25.00
ATOM	640	CE1	PHE	95	50.463	26.284	55.865	1.00	25.00
ATOM	641	CE2	PHE	95	51.863	28.058	55.083	1.00	25.00
ATOM	642	CZ	PHE	95	51.504	26.741	55.054	1.00	25.00
ATOM	645	N	GLY	96	46.404	30.213	59.121	1.00	25.00
ATOM	646	CA	GLY	96	45.871	31.140	60.103	1.00	25.00
ATOM	647	C	GLY	96	46.804	31.220	61.300	1.00	25.00
ATOM	648	O	GLY	96	47.991	30.885	61.200	1.00	25.00
ATOM	649	N	ASN	97	46.273	31.640	62.447	1.00	25.00
ATOM	650	CA	ASN	97	47.086	31.705	63.641	1.00	25.00
ATOM	655	C	ASN	97	47.012	30.350	64.285	1.00	25.00
ATOM	656	O	ASN	97	47.825	30.028	65.142	1.00	25.00
ATOM	651	CB	ASN	97	46.611	32.805	64.567	1.00	25.00
ATOM	652	CG	ASN	97	46.889	34.197	64.001	1.00	25.00
ATOM	653	OD1	ASN	97	48.046	34.569	63.779	1.00	25.00
ATOM	654	ND2	ASN	97	45.830	34.972	63.765	1.00	25.00
ATOM	657	N	ARG	98	46.074	29.528	63.815	1.00	25.00
ATOM	658	CA	ARG	98	45.920	28.169	64.328	1.00	25.00

Fig. 23S

ATOM	666	C	ARG	98	47.120	27.347	63.912	1.00	25.00
ATOM	667	O	ARG	98	47.328	26.230	64.399	1.00	25.00
ATOM	659	CB	ARG	98	44.625	27.502	63.834	1.00	25.00
ATOM	660	CG	ARG	98	44.302	27.658	62.354	1.00	25.00
ATOM	661	CD	ARG	98	43.187	26.694	61.875	1.00	25.00
ATOM	662	NE	ARG	98	43.725	25.367	61.594	1.00	25.00
ATOM	663	CZ	ARG	98	43.514	24.678	60.479	1.00	25.00
ATOM	664	NH1	ARG	98	42.730	25.170	59.537	1.00	25.00
ATOM	665	NH2	ARG	98	44.068	23.476	60.324	1.00	25.00
ATOM	668	N	ASP	99	47.870	27.915	62.967	1.00	25.00
ATOM	669	CA	ASP	99	49.089	27.326	62.427	1.00	25.00
ATOM	674	C	ASP	99	50.267	27.962	63.147	1.00	25.00
ATOM	675	O	ASP	99	51.250	27.291	63.455	1.00	25.00
ATOM	670	CB	ASP	99	49.187	27.556	60.918	1.00	25.00
ATOM	671	CG	ASP	99	48.066	26.886	60.159	1.00	25.00
ATOM	672	OD1	ASP	99	47.856	25.685	60.384	1.00	25.00
ATOM	673	OD2	ASP	99	47.379	27.554	59.357	1.00	25.00
ATOM	676	N	SER	100	50.165	29.256	63.431	1.00	25.00
ATOM	677	CA	SER	100	51.224	29.946	64.165	1.00	25.00
ATOM	680	C	SER	100	51.527	29.031	65.335	1.00	25.00
ATOM	681	O	SER	100	52.618	28.447	65.482	1.00	25.00
ATOM	678	CB	SER	100	50.741	31.307	64.721	1.00	25.00
ATOM	679	OG	SER	100	50.565	32.285	63.700	1.00	25.00
ATOM	682	N	VAL	101	50.479	28.758	66.072	1.00	25.00
ATOM	683	CA	VAL	101	50.674	27.923	67.222	1.00	25.00
ATOM	687	C	VAL	101	50.777	26.417	66.900	1.00	25.00
ATOM	688	O	VAL	101	50.062	25.598	67.506	1.00	25.00
ATOM	684	CB	VAL	101	49.645	28.277	68.355	1.00	25.00
ATOM	685	CG1	VAL	101	50.396	28.491	69.688	1.00	25.00
ATOM	686	CG2	VAL	101	48.859	29.570	67.983	1.00	25.00
ATOM	689	N	LEU	102	51.622	26.070	65.918	1.00	25.00
ATOM	690	CA	LEU	102	51.849	24.668	65.595	1.00	25.00
ATOM	695	C	LEU	102	52.763	24.244	64.446	1.00	25.00
ATOM	696	O	LEU	102	53.401	23.192	64.550	1.00	25.00
ATOM	691	CB	LEU	102	50.538	23.858	65.550	1.00	25.00
ATOM	692	CG	LEU	102	50.710	22.549	66.361	1.00	25.00
ATOM	693	CD1	LEU	102	51.013	22.854	67.857	1.00	25.00

Fig. 23T

ATOM	694	CD2	LEU	102	49.517	21.603	66.215	1.00	25.00
ATOM	697	N	SER	103	52.885	25.030	63.380	1.00	25.00
ATOM	698	CA	SER	103	53.717	24.611	62.242	1.00	25.00
ATOM	701	C	SER	103	55.014	25.434	62.112	1.00	25.00
ATOM	702	O	SER	103	55.002	26.622	62.399	1.00	25.00
ATOM	699	CB	SER	103	52.873	24.626	60.950	1.00	25.00
ATOM	700	OG	SER	103	51.778	23.711	61.012	1.00	25.00
ATOM	703	N	PRO	104	56.157	24.785	61.746	1.00	25.00
ATOM	705	CA	PRO	104	57.528	25.310	61.556	1.00	25.00
ATOM	708	C	PRO	104	58.286	25.311	60.201	1.00	25.00
ATOM	709	O	PRO	104	58.997	26.272	59.897	1.00	25.00
ATOM	706	CB	PRO	104	58.302	24.457	62.542	1.00	25.00
ATOM	707	CG	PRO	104	57.703	23.081	62.303	1.00	25.00
ATOM	704	CD	PRO	104	56.214	23.356	62.109	1.00	25.00
ATOM	710	N	LEU	105	58.340	24.113	59.593	1.00	25.00
ATOM	711	CA	LEU	105	58.967	23.714	58.307	1.00	25.00
ATOM	716	C	LEU	105	57.880	22.827	57.685	1.00	25.00
ATOM	717	O	LEU	105	57.965	22.402	56.532	1.00	25.00
ATOM	712	CB	LEU	105	60.191	22.812	58.567	1.00	25.00
ATOM	713	CG	LEU	105	60.481	21.572	57.686	1.00	25.00
ATOM	714	CD1	LEU	105	61.539	21.918	56.706	1.00	25.00
ATOM	715	CD2	LEU	105	60.965	20.370	58.457	1.00	25.00
ATOM	718	N	GLU	106	56.881	22.488	58.502	1.00	25.00
ATOM	719	CA	GLU	106	55.730	21.694	58.086	1.00	25.00
ATOM	725	C	GLU	106	54.897	22.621	57.220	1.00	25.00
ATOM	726	O	GLU	106	53.960	22.200	56.555	1.00	25.00
ATOM	720	CB	GLU	106	54.939	21.264	59.312	1.00	25.00
ATOM	721	CG	GLU	106	55.821	20.599	60.344	1.00	25.00
ATOM	722	CD	GLU	106	55.087	20.260	61.602	1.00	25.00
ATOM	723	OE1	GLU	106	54.316	21.121	62.080	1.00	25.00
ATOM	724	OE2	GLU	106	55.291	19.132	62.108	1.00	25.00
ATOM	727	N	ARG	107	55.224	23.904	57.294	1.00	25.00
ATOM	728	CA	ARG	107	54.579	24.904	56.500	1.00	25.00
ATOM	736	C	ARG	107	55.199	24.880	55.104	1.00	25.00
ATOM	737	O	ARG	107	54.539	25.224	54.129	1.00	25.00
ATOM	729	CB	ARG	107	54.722	26.260	57.162	1.00	25.00
ATOM	730	CG	ARG	107	53.923	26.337	58.441	1.00	25.00

Fig. 23U

ATOM	731	CD	ARG	107	53.468	27.742	58.744	1.00	25.00
ATOM	732	NE	ARG	107	54.365	28.401	59.675	1.00	25.00
ATOM	733	CZ	ARG	107	53.995	28.838	60.878	1.00	25.00
ATOM	734	NH1	ARG	107	52.725	28.708	61.264	1.00	25.00
ATOM	735	NH2	ARG	107	54.888	29.426	61.688	1.00	25.00
ATOM	738	N	ALA	108	56.447	24.431	54.992	1.00	25.00
ATOM	739	CA	ALA	108	57.105	24.339	53.690	1.00	25.00
ATOM	741	C	ALA	108	56.434	23.172	53.071	1.00	25.00
ATOM	742	O	ALA	108	55.887	23.264	51.994	1.00	25.00
ATOM	740	CB	ALA	108	58.585	24.025	53.839	1.00	25.00
ATOM	743	N	LEU	109	56.432	22.085	53.823	1.00	25.00
ATOM	744	CA	LEU	109	55.831	20.839	53.399	1.00	25.00
ATOM	749	C	LEU	109	54.389	20.992	52.955	1.00	25.00
ATOM	750	O	LEU	109	53.976	20.346	52.019	1.00	25.00
ATOM	745	CB	LEU	109	55.925	19.816	54.525	1.00	25.00
ATOM	746	CG	LEU	109	55.682	18.345	54.210	1.00	25.00
ATOM	747	CD1	LEU	109	56.666	17.856	53.193	1.00	25.00
ATOM	748	CD2	LEU	109	55.854	17.572	55.470	1.00	25.00
ATOM	751	N	TYR	110	53.620	21.838	53.626	1.00	25.00
ATOM	752	CA	TYR	110	52.212	22.071	53.275	1.00	25.00
ATOM	761	C	TYR	110	52.057	22.737	51.920	1.00	25.00
ATOM	762	O	TYR	110	51.091	22.463	51.209	1.00	25.00
ATOM	753	CB	TYR	110	51.511	22.940	54.333	1.00	25.00
ATOM	754	CG	TYR	110	50.090	23.264	53.973	1.00	25.00
ATOM	755	CD1	TYR	110	49.791	24.352	53.169	1.00	25.00
ATOM	757	CD2	TYR	110	49.052	22.449	54.386	1.00	25.00
ATOM	756	CE1	TYR	110	48.494	24.618	52.780	1.00	25.00
ATOM	758	CE2	TYR	110	47.746	22.702	54.006	1.00	25.00
ATOM	759	CZ	TYR	110	47.473	23.791	53.199	1.00	25.00
ATOM	760	OH	TYR	110	46.176	24.054	52.810	1.00	25.00
ATOM	763	N	LEU	111	52.951	23.690	51.633	1.00	25.00
ATOM	764	CA	LEU	111	52.988	24.442	50.376	1.00	25.00
ATOM	769	C	LEU	111	53.417	23.567	49.194	1.00	25.00
ATOM	770	O	LEU	111	52.764	23.554	48.156	1.00	25.00
ATOM	765	CB	LEU	111	53.974	25.609	50.491	1.00	25.00
ATOM	766	CG	LEU	111	53.575	27.030	50.874	1.00	25.00
ATOM	767	CD1	LEU	111	52.258	27.384	50.228	1.00	25.00

Fig. 23V

ATOM	768	CD2	LEU	111	53.484	27.175	52.340	1.00	25.00
ATOM	771	N	VAL	112	54.528	22.852	49.365	1.00	25.00
ATOM	772	CA	VAL	112	55.088	21.988	48.330	1.00	25.00
ATOM	776	C	VAL	112	54.212	20.805	47.971	1.00	25.00
ATOM	777	O	VAL	112	54.215	20.372	46.813	1.00	25.00
ATOM	773	CB	VAL	112	56.512	21.489	48.678	1.00	25.00
ATOM	774	CG1	VAL	112	56.489	20.680	49.912	1.00	25.00
ATOM	775	CG2	VAL	112	57.067	20.659	47.563	1.00	25.00
ATOM	778	N	THR	113	53.461	20.284	48.940	1.00	25.00
ATOM	779	CA	THR	113	52.593	19.154	48.665	1.00	25.00
ATOM	783	C	THR	113	51.431	19.606	47.819	1.00	25.00
ATOM	784	O	THR	113	51.114	18.948	46.857	1.00	25.00
ATOM	780	CB	THR	113	52.074	18.439	49.935	1.00	25.00
ATOM	781	OG1	THR	113	53.166	17.858	50.638	1.00	25.00
ATOM	782	CG2	THR	113	51.169	17.311	49.573	1.00	25.00
ATOM	785	N	ASN	114	50.840	20.755	48.116	1.00	25.00
ATOM	786	CA	ASN	114	49.699	21.197	47.326	1.00	25.00
ATOM	791	C	ASN	114	50.020	21.818	45.961	1.00	25.00
ATOM	792	O	ASN	114	49.209	21.734	45.032	1.00	25.00
ATOM	787	CB	ASN	114	48.794	22.113	48.145	1.00	25.00
ATOM	788	CG	ASN	114	47.927	21.352	49.131	1.00	25.00
ATOM	789	OD1	ASN	114	46.785	21.007	48.841	1.00	25.00
ATOM	790	ND2	ASN	114	48.458	21.109	50.307	1.00	25.00
ATOM	793	N	TYR	115	51.197	22.427	45.831	1.00	25.00
ATOM	794	CA	TYR	115	51.618	23.039	44.561	1.00	25.00
ATOM	803	C	TYR	115	52.119	21.984	43.567	1.00	25.00
ATOM	804	O	TYR	115	51.715	21.989	42.417	1.00	25.00
ATOM	795	CB	TYR	115	52.729	24.077	44.792	1.00	25.00
ATOM	796	CG	TYR	115	52.859	25.101	43.677	1.00	25.00
ATOM	797	CD1	TYR	115	53.635	24.854	42.552	1.00	25.00
ATOM	799	CD2	TYR	115	52.123	26.280	43.713	1.00	25.00
ATOM	798	CE1	TYR	115	53.658	25.748	41.494	1.00	25.00
ATOM	800	CE2	TYR	115	52.141	27.167	42.666	1.00	25.00
ATOM	801	CZ	TYR	115	52.901	26.893	41.560	1.00	25.00
ATOM	802	OH	TYR	115	52.844	27.764	40.513	1.00	25.00
ATOM	805	N	LEU	116	52.985	21.082	44.033	1.00	25.00
ATOM	806	CA	LEU	116	53.574	20.023	43.220	1.00	25.00

Fig. 23W

ATOM	811	C	LEU	116	53.167	18.605	43.661	1.00	25.00
ATOM	812	O	LEU	116	54.016	17.803	44.029	1.00	25.00
ATOM	807	CB	LEU	116	55.083	20.134	43.325	1.00	25.00
ATOM	808	CG	LEU	116	55.741	21.400	42.807	1.00	25.00
ATOM	809	CD1	LEU	116	57.235	21.350	43.086	1.00	25.00
ATOM	810	CD2	LEU	116	55.469	21.513	41.324	1.00	25.00
ATOM	813	N	PRO	117	51.884	18.245	43.530	1.00	25.00
ATOM	815	CA	PRO	117	51.456	16.919	43.949	1.00	25.00
ATOM	818	C	PRO	117	51.861	15.676	43.202	1.00	25.00
ATOM	819	O	PRO	117	51.764	14.600	43.766	1.00	25.00
ATOM	816	CB	PRO	117	49.938	17.056	44.026	1.00	25.00
ATOM	817	CG	PRO	117	49.624	18.054	43.036	1.00	25.00
ATOM	814	CD	PRO	117	50.716	19.075	43.198	1.00	25.00
ATOM	820	N	SER	118	52.267	15.765	41.949	1.00	25.00
ATOM	821	CA	SER	118	52.647	14.547	41.241	1.00	25.00
ATOM	824	C	SER	118	54.125	14.431	40.822	1.00	25.00
ATOM	825	O	SER	118	54.892	15.393	40.879	1.00	25.00
ATOM	822	CB	SER	118	51.709	14.303	40.055	1.00	25.00
ATOM	823	OG	SER	118	50.344	14.223	40.459	1.00	25.00
ATOM	826	N	VAL	119	54.511	13.236	40.390	1.00	25.00
ATOM	827	CA	VAL	119	55.880	12.925	39.984	1.00	25.00
ATOM	831	C	VAL	119	55.861	12.316	38.608	1.00	25.00
ATOM	832	O	VAL	119	55.075	11.411	38.369	1.00	25.00
ATOM	828	CB	VAL	119	56.488	11.905	40.950	1.00	25.00
ATOM	829	CG1	VAL	119	57.342	10.846	40.207	1.00	25.00
ATOM	830	CG2	VAL	119	57.275	12.650	42.051	1.00	25.00
ATOM	833	N	SER	120	56.783	12.750	37.744	1.00	25.00
ATOM	834	CA	SER	120	56.871	12.264	36.371	1.00	25.00
ATOM	837	C	SER	120	58.207	11.615	36.106	1.00	25.00
ATOM	838	O	SER	120	59.223	12.257	36.207	1.00	25.00
ATOM	835	CB	SER	120	56.654	13.416	35.393	1.00	25.00
ATOM	836	OG	SER	120	55.882	13.005	34.260	1.00	25.00
ATOM	839	N	LEU	121	58.187	10.328	35.782	1.00	25.00
ATOM	840	CA	LEU	121	59.395	9.548	35.501	1.00	25.00
ATOM	845	C	LEU	121	59.784	9.666	34.055	1.00	25.00
ATOM	846	O	LEU	121	59.252	8.937	33.211	1.00	25.00
ATOM	841	CB	LEU	121	59.149	8.062	35.769	1.00	25.00

Fig. 23X

ATOM	842	CG	LEU	121	60.287	7.140	35.336	1.00	25.00
ATOM	843	CD1	LEU	121	61.467	7.267	36.274	1.00	25.00
ATOM	844	CD2	LEU	121	59.808	5.728	35.309	1.00	25.00
ATOM	847	N	SER	122	60.685	10.577	33.743	1.00	25.00
ATOM	848	CA	SER	122	61.107	10.697	32.356	1.00	25.00
ATOM	851	C	SER	122	62.017	9.485	32.133	1.00	25.00
ATOM	852	O	SER	122	63.223	9.520	32.442	1.00	25.00
ATOM	849	CB	SER	122	61.864	12.007	32.113	1.00	25.00
ATOM	850	OG	SER	122	61.773	12.871	33.244	1.00	25.00
ATOM	853	N	SER	123	61.401	8.370	31.748	1.00	25.00
ATOM	854	CA	SER	123	62.147	7.150	31.515	1.00	25.00
ATOM	857	C	SER	123	62.965	7.427	30.296	1.00	25.00
ATOM	858	O	SER	123	62.572	8.252	29.473	1.00	25.00
ATOM	855	CB	SER	123	61.202	5.983	31.233	1.00	25.00
ATOM	856	OG	SER	123	61.923	4.755	31.199	1.00	25.00
ATOM	859	N	LYS	124	64.152	6.847	30.237	1.00	25.00
ATOM	860	CA	LYS	124	65.000	7.032	29.061	1.00	25.00
ATOM	866	C	LYS	124	64.725	5.781	28.237	1.00	25.00
ATOM	867	O	LYS	124	64.801	5.774	26.992	1.00	25.00
ATOM	861	CB	LYS	124	66.481	7.083	29.464	1.00	25.00
ATOM	862	CG	LYS	124	67.400	7.815	28.484	1.00	25.00
ATOM	863	CD	LYS	124	68.833	7.365	28.701	1.00	25.00
ATOM	864	CE	LYS	124	68.925	5.848	28.543	1.00	25.00
ATOM	865	NZ	LYS	124	68.304	5.370	27.255	1.00	25.00
ATOM	868	N	ARG	125	64.314	4.774	29.004	1.00	25.00
ATOM	869	CA	ARG	125	63.969	3.404	28.620	1.00	25.00
ATOM	871	C	ARG	125	64.089	2.840	30.011	1.00	25.00
ATOM	872	O	ARG	125	63.215	2.138	30.531	1.00	25.00
ATOM	870	CB	ARG	125	65.053	2.799	27.745	1.00	25.00
ATOM	873	N	LEU	126	65.161	3.329	30.616	1.00	25.00
ATOM	874	CA	LEU	126	65.609	3.058	31.953	1.00	25.00
ATOM	876	C	LEU	126	66.889	3.904	31.936	1.00	25.00
ATOM	877	O	LEU	126	67.979	3.412	32.317	1.00	25.00
ATOM	875	CB	LEU	126	65.934	1.578	32.123	1.00	25.00
ATOM	878	OT	LEU	126	66.774	5.077	31.502	1.00	25.00
ATOM	888	N	PHE	137	67.101	5.496	34.406	1.00	25.00
ATOM	889	CA	PHE	137	65.776	6.051	34.080	1.00	25.00

Fig. 23Y

ATOM	886	C	PHE	137	65.966	7.381	33.389	1.00	25.00
ATOM	887	O	PHE	137	65.563	7.531	32.239	1.00	25.00
ATOM	879	CB	PHE	137	64.934	6.181	35.332	1.00	25.00
ATOM	880	CG	PHE	137	64.182	4.925	35.682	1.00	25.00
ATOM	881	CD1	PHE	137	63.514	4.199	34.693	1.00	25.00
ATOM	882	CD2	PHE	137	64.123	4.467	36.999	1.00	25.00
ATOM	883	CE1	PHE	137	62.796	3.035	35.017	1.00	25.00
ATOM	884	CE2	PHE	137	63.413	3.314	37.320	1.00	25.00
ATOM	885	CZ	PHE	137	62.748	2.599	36.326	1.00	25.00
ATOM	890	N	THR	138	66.627	8.304	34.092	1.00	25.00
ATOM	891	CA	THR	138	66.975	9.675	33.669	1.00	25.00
ATOM	895	C	THR	138	66.660	10.618	34.832	1.00	25.00
ATOM	896	O	THR	138	67.551	10.903	35.648	1.00	25.00
ATOM	892	CB	THR	138	66.330	10.132	32.324	1.00	25.00
ATOM	893	OG1	THR	138	66.990	9.472	31.241	1.00	25.00
ATOM	894	CG2	THR	138	66.518	11.601	32.106	1.00	25.00
ATOM	897	N	HIS	139	65.401	11.038	34.964	1.00	25.00
ATOM	898	CA	HIS	139	65.038	11.906	36.075	1.00	25.00
ATOM	899	C	HIS	139	63.544	11.855	36.391	1.00	25.00
ATOM	900	O	HIS	139	62.740	11.480	35.530	1.00	25.00
ATOM	901	CB	HIS	139	65.484	13.338	35.810	1.00	25.00
ATOM	902	CG	HIS	139	64.651	14.035	34.794	1.00	25.00
ATOM	903	ND1	HIS	139	63.791	15.068	35.084	1.00	25.00
ATOM	904	CD2	HIS	139	64.485	13.778	33.477	1.00	25.00
ATOM	906	CE1	HIS	139	63.141	15.388	33.977	1.00	25.00
ATOM	905	NE2	HIS	139	63.529	14.632	32.974	1.00	25.00
ATOM	907	N	VAL	140	63.221	12.183	37.648	1.00	25.00
ATOM	908	CA	VAL	140	61.871	12.220	38.222	1.00	25.00
ATOM	912	C	VAL	140	61.445	13.693	38.300	1.00	25.00
ATOM	913	O	VAL	140	62.134	14.486	38.943	1.00	25.00
ATOM	909	CB	VAL	140	61.906	11.666	39.684	1.00	25.00
ATOM	910	CG1	VAL	140	60.629	12.001	40.424	1.00	25.00
ATOM	911	CG2	VAL	140	62.174	10.151	39.681	1.00	25.00
ATOM	914	N	ALA	141	60.318	14.066	37.692	1.00	25.00
ATOM	915	CA	ALA	141	59.858	15.448	37.716	1.00	25.00
ATOM	917	C	ALA	141	58.722	15.656	38.716	1.00	25.00
ATOM	918	O	ALA	141	57.934	14.758	38.967	1.00	25.00

Fig. 232

ATOM	916	CB	ALA	141	59.413	15.840	36.364	1.00	25.00
ATOM	919	N	LEU	142	58.688	16.810	39.359	1.00	25.00
ATOM	920	CA	LEU	142	57.604	17.110	40.281	1.00	25.00
ATOM	925	C	LEU	142	56.659	17.994	39.450	1.00	25.00
ATOM	926	O	LEU	142	57.124	18.839	38.696	1.00	25.00
ATOM	921	CB	LEU	142	58.125	17.851	41.528	1.00	25.00
ATOM	922	CG	LEU	142	59.034	17.139	42.551	1.00	25.00
ATOM	923	CD1	LEU	142	59.343	18.104	43.664	1.00	25.00
ATOM	924	CD2	LEU	142	58.405	15.865	43.103	1.00	25.00
ATOM	927	N	CYS	143	55.349	17.841	39.601	1.00	25.00
ATOM	928	CA	CYS	143	54.419	18.608	38.783	1.00	25.00
ATOM	931	C	CYS	143	53.004	18.555	39.358	1.00	25.00
ATOM	932	O	CYS	143	52.801	17.928	40.375	1.00	25.00
ATOM	929	CB	CYS	143	54.426	17.953	37.403	1.00	25.00
ATOM	930	SG	CYS	143	54.272	16.114	37.477	1.00	25.00
ATOM	933	N	VAL	144	52.026	19.207	38.723	1.00	25.00
ATOM	934	CA	VAL	144	50.644	19.138	39.206	1.00	25.00
ATOM	938	C	VAL	144	50.171	17.696	39.058	1.00	25.00
ATOM	939	O	VAL	144	50.033	16.976	40.045	1.00	25.00
ATOM	935	CB	VAL	144	49.712	20.056	38.431	1.00	25.00
ATOM	936	CG1	VAL	144	48.256	19.803	38.800	1.00	25.00
ATOM	937	CG2	VAL	144	50.053	21.459	38.754	1.00	25.00
ATOM	940	N	VAL	145	49.916	17.257	37.833	1.00	25.00
ATOM	941	CA	VAL	145	49.504	15.879	37.633	1.00	25.00
ATOM	945	C	VAL	145	50.315	15.299	36.508	1.00	25.00
ATOM	946	O	VAL	145	50.699	16.007	35.580	1.00	25.00
ATOM	942	CB	VAL	145	48.029	15.746	37.337	1.00	25.00
ATOM	943	CG1	VAL	145	47.246	16.718	38.216	1.00	25.00
ATOM	944	CG2	VAL	145	47.752	15.906	35.850	1.00	25.00
ATOM	947	N	GLY	146	50.620	14.017	36.618	1.00	25.00
ATOM	948	CA	GLY	146	51.419	13.379	35.596	1.00	25.00
ATOM	949	C	GLY	146	50.620	12.610	34.570	1.00	25.00
ATOM	950	O	GLY	146	49.427	12.353	34.722	1.00	25.00
ATOM	951	N	ARG	147	51.312	12.231	33.512	1.00	25.00
ATOM	952	CA	ARG	147	50.733	11.463	32.422	1.00	25.00
ATOM	960	C	ARG	147	50.256	10.082	32.917	1.00	25.00
ATOM	961	O	ARG	147	49.302	9.523	32.355	1.00	25.00

Fig. 23AA

ATOM	953	CB	ARG	147	51.807	11.235	31.366	1.00	25.00
ATOM	954	CG	ARG	147	52.970	12.230	31.429	1.00	25.00
ATOM	955	CD	ARG	147	52.760	13.360	30.428	1.00	25.00
ATOM	956	NE	ARG	147	52.455	12.799	29.116	1.00	25.00
ATOM	957	CZ	ARG	147	53.210	11.894	28.492	1.00	25.00
ATOM	958	NH1	ARG	147	54.375	11.489	29.014	1.00	25.00
ATOM	959	NH2	ARG	147	52.815	11.430	27.314	1.00	25.00
ATOM	962	N	ARG	148	50.936	9.527	33.937	1.00	25.00
ATOM	963	CA	ARG	148	50.619	8.200	34.492	1.00	25.00
ATOM	971	C	ARG	148	49.540	8.123	35.562	1.00	25.00
ATOM	972	O	ARG	148	49.295	9.085	36.276	1.00	25.00
ATOM	964	CB	ARG	148	51.899	7.483	34.904	1.00	25.00
ATOM	965	CG	ARG	148	52.654	7.052	33.662	1.00	25.00
ATOM	966	CD	ARG	148	54.099	6.580	33.847	1.00	25.00
ATOM	967	NE	ARG	148	54.697	6.425	32.515	1.00	25.00
ATOM	968	CZ	ARG	148	55.985	6.252	32.253	1.00	25.00
ATOM	969	NH1	ARG	148	56.888	6.174	33.227	1.00	25.00
ATOM	970	NH2	ARG	148	56.356	6.145	30.987	1.00	25.00
ATOM	973	N	VAL	149	48.965	6.939	35.731	1.00	25.00
ATOM	974	CA	VAL	149	47.837	6.753	36.644	1.00	25.00
ATOM	978	C	VAL	149	47.912	6.676	38.183	1.00	25.00
ATOM	979	O	VAL	149	46.872	6.800	38.838	1.00	25.00
ATOM	975	CB	VAL	149	46.903	5.615	36.126	1.00	25.00
ATOM	976	CG1	VAL	149	46.581	5.836	34.653	1.00	25.00
ATOM	977	CG2	VAL	149	47.541	4.250	36.351	1.00	25.00
ATOM	980	N	GLY	150	49.065	6.409	38.780	1.00	25.00
ATOM	981	CA	GLY	150	49.101	6.364	40.240	1.00	25.00
ATOM	982	C	GLY	150	50.180	7.311	40.742	1.00	25.00
ATOM	983	O	GLY	150	50.622	7.207	41.900	1.00	25.00
ATOM	984	N	THR	151	50.556	8.258	39.865	1.00	25.00
ATOM	985	CA	THR	151	51.633	9.217	40.098	1.00	25.00
ATOM	989	C	THR	151	51.434	10.313	41.121	1.00	25.00
ATOM	990	O	THR	151	52.115	11.327	41.056	1.00	25.00
ATOM	986	CB	THR	151	52.147	9.874	38.776	1.00	25.00
ATOM	987	OG1	THR	151	51.071	10.519	38.077	1.00	25.00
ATOM	988	CG2	THR	151	52.809	8.866	37.871	1.00	25.00
ATOM	991	N	VAL	152	50.487	10.166	42.038	1.00	25.00

Fig. 23BB

ATOM	992	CA	VAL	152	50.334	11.182	43.072	1.00	25.00
ATOM	996	C	VAL	152	51.399	10.842	44.134	1.00	25.00
ATOM	997	O	VAL	152	51.763	9.670	44.302	1.00	25.00
ATOM	993	CB	VAL	152	48.916	11.189	43.628	1.00	25.00
ATOM	994	CG1	VAL	152	48.928	11.304	45.114	1.00	25.00
ATOM	995	CG2	VAL	152	48.159	12.342	43.036	1.00	25.00
ATOM	998	N	VAL	153	51.967	11.842	44.793	1.00	25.00
ATOM	999	CA	VAL	153	52.989	11.544	45.778	1.00	25.00
ATOM	1003	C	VAL	153	52.737	12.086	47.168	1.00	25.00
ATOM	1004	O	VAL	153	51.866	12.917	47.367	1.00	25.00
ATOM	1000	CB	VAL	153	54.382	11.975	45.306	1.00	25.00
ATOM	1001	CG1	VAL	153	54.834	11.087	44.207	1.00	25.00
ATOM	1002	CG2	VAL	153	54.377	13.397	44.871	1.00	25.00
ATOM	1005	N	ASN	154	53.473	11.551	48.135	1.00	25.00
ATOM	1006	CA	ASN	154	53.382	11.978	49.508	1.00	25.00
ATOM	1011	C	ASN	154	54.757	12.511	49.882	1.00	25.00
ATOM	1012	O	ASN	154	55.777	12.012	49.408	1.00	25.00
ATOM	1007	CB	ASN	154	52.972	10.815	50.406	1.00	25.00
ATOM	1008	CG	ASN	154	52.574	11.261	51.805	1.00	25.00
ATOM	1009	OD1	ASN	154	51.682	12.084	51.980	1.00	25.00
ATOM	1010	ND2	ASN	154	53.230	10.704	52.812	1.00	25.00
ATOM	1013	N	TYR	155	54.751	13.599	50.646	1.00	25.00
ATOM	1014	CA	TYR	155	55.943	14.294	51.140	1.00	25.00
ATOM	1023	C	TYR	155	55.826	14.353	52.664	1.00	25.00
ATOM	1024	O	TYR	155	54.714	14.502	53.184	1.00	25.00
ATOM	1015	CB	TYR	155	55.942	15.761	50.700	1.00	25.00
ATOM	1016	CG	TYR	155	56.046	16.082	49.237	1.00	25.00
ATOM	1017	CD1	TYR	155	54.952	15.954	48.390	1.00	25.00
ATOM	1019	CD2	TYR	155	57.222	16.604	48.722	1.00	25.00
ATOM	1018	CE1	TYR	155	55.027	16.341	47.055	1.00	25.00
ATOM	1020	CE2	TYR	155	57.316	16.997	47.398	1.00	25.00
ATOM	1021	CZ	TYR	155	56.218	16.865	46.555	1.00	25.00
ATOM	1022	OH	TYR	155	56.341	17.235	45.223	1.00	25.00
ATOM	1025	N	ASP	156	56.953	14.260	53.369	1.00	25.00
ATOM	1026	CA	ASP	156	56.976	14.369	54.841	1.00	25.00
ATOM	1031	C	ASP	156	58.388	14.641	55.289	1.00	25.00
ATOM	1032	O	ASP	156	59.268	14.776	54.444	1.00	25.00

Fig. 23CC

ATOM	1027	CB	ASP	156	56.469	13.116	55.549	1.00	25.00
ATOM	1028	CG	ASP	156	55.697	13.439	56.813	1.00	25.00
ATOM	1029	OD1	ASP	156	55.994	14.431	57.485	1.00	25.00
ATOM	1030	OD2	ASP	156	54.757	12.709	57.127	1.00	25.00
ATOM	1033	N	CYS	157	58.642	14.668	56.591	1.00	25.00
ATOM	1034	CA	CYS	157	59.997	14.951	57.027	1.00	25.00
ATOM	1037	C	CYS	157	60.814	13.822	57.600	1.00	25.00
ATOM	1038	O	CYS	157	61.688	14.071	58.410	1.00	25.00
ATOM	1035	CB	CYS	157	60.042	16.145	57.964	1.00	25.00
ATOM	1036	SG	CYS	157	58.432	16.648	58.447	1.00	25.00
ATOM	1039	N	THR	158	60.552	12.595	57.174	1.00	25.00
ATOM	1040	CA	THR	158	61.305	11.433	57.621	1.00	25.00
ATOM	1044	C	THR	158	60.948	10.358	56.611	1.00	25.00
ATOM	1045	O	THR	158	59.770	10.180	56.296	1.00	25.00
ATOM	1041	CB	THR	158	60.813	10.918	58.957	1.00	25.00
ATOM	1042	OG1	THR	158	59.453	10.518	58.808	1.00	25.00
ATOM	1043	CG2	THR	158	60.912	11.961	60.040	1.00	25.00
ATOM	1046	N	PRO	159	61.929	9.585	56.134	1.00	25.00
ATOM	1048	CA	PRO	159	61.620	8.545	55.160	1.00	25.00
ATOM	1051	C	PRO	159	60.461	7.627	55.538	1.00	25.00
ATOM	1052	O	PRO	159	59.575	7.374	54.718	1.00	25.00
ATOM	1049	CB	PRO	159	62.927	7.780	55.063	1.00	25.00
ATOM	1050	CG	PRO	159	63.523	7.997	56.363	1.00	25.00
ATOM	1047	CD	PRO	159	63.311	9.452	56.578	1.00	25.00
ATOM	1053	N	GLU	160	60.416	7.179	56.790	1.00	25.00
ATOM	1054	CA	GLU	160	59.354	6.265	57.196	1.00	25.00
ATOM	1060	C	GLU	160	57.981	6.903	57.232	1.00	25.00
ATOM	1061	O	GLU	160	56.988	6.197	57.364	1.00	25.00
ATOM	1055	CB	GLU	160	59.663	5.583	58.524	1.00	25.00
ATOM	1056	CG	GLU	160	59.432	6.450	59.731	1.00	25.00
ATOM	1057	CD	GLU	160	60.662	7.233	60.149	1.00	25.00
ATOM	1058	OE1	GLU	160	61.643	7.272	59.364	1.00	25.00
ATOM	1059	OE2	GLU	160	60.643	7.793	61.280	1.00	25.00
ATOM	1062	N	SER	161	57.915	8.226	57.113	1.00	25.00
ATOM	1063	CA	SER	161	56.633	8.923	57.115	1.00	25.00
ATOM	1066	C	SER	161	56.107	9.213	55.716	1.00	25.00
ATOM	1067	O	SER	161	54.896	9.368	55.510	1.00	25.00

Fig. 23DD

ATOM	1064	CB	SER	161	56.739	10.211	57.887	1.00	25.00
ATOM	1065	OG	SER	161	57.021	9.902	59.222	1.00	25.00
ATOM	1068	N	SER	162	57.011	9.313	54.756	1.00	25.00
ATOM	1069	CA	SER	162	56.625	9.580	53.392	1.00	25.00
ATOM	1072	C	SER	162	55.901	8.360	52.904	1.00	25.00
ATOM	1073	O	SER	162	54.863	8.453	52.269	1.00	25.00
ATOM	1070	CB	SER	162	57.879	9.781	52.600	1.00	25.00
ATOM	1071	OG	SER	162	58.729	10.607	53.368	1.00	25.00
ATOM	1074	N	ILE	163	56.416	7.209	53.305	1.00	25.00
ATOM	1075	CA	ILE	163	55.856	5.931	52.915	1.00	25.00
ATOM	1080	C	ILE	163	54.836	5.381	53.882	1.00	25.00
ATOM	1081	O	ILE	163	54.152	4.414	53.570	1.00	25.00
ATOM	1076	CB	ILE	163	56.945	4.861	52.775	1.00	25.00
ATOM	1078	CG1	ILE	163	57.626	4.619	54.122	1.00	25.00
ATOM	1077	CG2	ILE	163	57.962	5.276	51.725	1.00	25.00
ATOM	1079	CD1	ILE	163	58.610	3.481	54.075	1.00	25.00
ATOM	1082	N	GLU	164	54.723	5.978	55.052	1.00	25.00
ATOM	1083	CA	GLU	164	53.777	5.470	56.017	1.00	25.00
ATOM	1089	C	GLU	164	52.304	5.326	55.586	1.00	25.00
ATOM	1090	O	GLU	164	51.645	4.360	56.004	1.00	25.00
ATOM	1084	CB	GLU	164	53.864	6.264	57.292	1.00	25.00
ATOM	1085	CG	GLU	164	53.019	5.667	58.342	1.00	25.00
ATOM	1086	CD	GLU	164	52.542	6.682	59.328	1.00	25.00
ATOM	1087	OE1	GLU	164	51.816	7.611	58.892	1.00	25.00
ATOM	1088	OE2	GLU	164	52.880	6.541	60.531	1.00	25.00
ATOM	1091	N	PRO	165	51.758	6.286	54.778	1.00	25.00
ATOM	1093	CA	PRO	165	50.366	6.298	54.276	1.00	25.00
ATOM	1096	C	PRO	165	49.918	5.425	53.107	1.00	25.00
ATOM	1097	O	PRO	165	48.737	5.447	52.771	1.00	25.00
ATOM	1094	CB	PRO	165	50.136	7.769	53.944	1.00	25.00
ATOM	1095	CG	PRO	165	51.471	8.224	53.512	1.00	25.00
ATOM	1092	CD	PRO	165	52.369	7.617	54.559	1.00	25.00
ATOM	1098	N	PHE	166	50.832	4.731	52.436	1.00	25.00
ATOM	1099	CA	PHE	166	50.454	3.855	51.324	1.00	25.00
ATOM	1107	C	PHE	166	49.900	2.574	51.927	1.00	25.00
ATOM	1108	O	PHE	166	50.667	1.677	52.240	1.00	25.00
ATOM	1100	CB	PHE	166	51.677	3.542	50.478	1.00	25.00

Fig. 23EE

ATOM	1101	CG	PHE	166	52.235	4.741	49.783	1.00	25.00
ATOM	1102	CD1	PHE	166	51.735	5.136	48.552	1.00	25.00
ATOM	1103	CD2	PHE	166	53.194	5.533	50.398	1.00	25.00
ATOM	1104	CE1	PHE	166	52.164	6.290	47.961	1.00	25.00
ATOM	1105	CE2	PHE	166	53.628	6.696	49.803	1.00	25.00
ATOM	1106	CZ	PHE	166	53.109	7.074	48.584	1.00	25.00
ATOM	1109	N	ARG	167	48.574	2.473	52.057	1.00	25.00
ATOM	1110	CA	ARG	167	47.919	1.316	52.690	1.00	25.00
ATOM	1118	C	ARG	167	48.110	-0.065	52.107	1.00	25.00
ATOM	1119	O	ARG	167	47.870	-1.060	52.784	1.00	25.00
ATOM	1111	CB	ARG	167	46.429	1.575	52.863	1.00	25.00
ATOM	1112	CG	ARG	167	46.076	2.858	53.645	1.00	25.00
ATOM	1113	CD	ARG	167	44.629	2.776	54.155	1.00	25.00
ATOM	1114	NE	ARG	167	44.004	4.075	54.430	1.00	25.00
ATOM	1115	CZ	ARG	167	42.778	4.221	54.942	1.00	25.00
ATOM	1116	NH1	ARG	167	42.053	3.145	55.252	1.00	25.00
ATOM	1117	NH2	ARG	167	42.273	5.435	55.155	1.00	25.00
ATOM	1120	N	VAL	168	48.489	-0.117	50.836	1.00	25.00
ATOM	1121	CA	VAL	168	48.726	-1.387	50.131	1.00	25.00
ATOM	1125	C	VAL	168	50.198	-1.862	50.180	1.00	25.00
ATOM	1126	O	VAL	168	50.477	-3.065	50.210	1.00	25.00
ATOM	1122	CB	VAL	168	48.268	-1.317	48.630	1.00	25.00
ATOM	1123	CG1	VAL	168	46.749	-1.167	48.539	1.00	25.00
ATOM	1124	CG2	VAL	168	48.969	-0.142	47.912	1.00	25.00
ATOM	1127	N	LEU	169	51.127	-0.913	50.189	1.00	25.00
ATOM	1128	CA	LEU	169	52.543	-1.221	50.220	1.00	25.00
ATOM	1133	C	LEU	169	52.869	-2.113	51.417	1.00	25.00
ATOM	1134	O	LEU	169	52.660	-1.746	52.561	1.00	25.00
ATOM	1129	CB	LEU	169	53.350	0.077	50.264	1.00	25.00
ATOM	1130	CG	LEU	169	54.850	-0.097	50.078	1.00	25.00
ATOM	1131	CD1	LEU	169	55.100	-0.596	48.667	1.00	25.00
ATOM	1132	CD2	LEU	169	55.604	1.192	50.366	1.00	25.00
ATOM	1135	N	SER	170	53.372	-3.299	51.127	1.00	25.00
ATOM	1136	CA	SER	170	53.734	-4.288	52.135	1.00	25.00
ATOM	1139	C	SER	170	54.730	-3.769	53.153	1.00	25.00
ATOM	1140	O	SER	170	55.620	-2.983	52.816	1.00	25.00
ATOM	1137	CB	SER	170	54.378	-5.486	51.448	1.00	25.00

Fig. 23FF

ATOM	1138	OG	SER	170	55.558	-5.087	50.768	1.00	25.00
ATOM	1141	N	MET	171	54.622	-4.260	54.386	1.00	25.00
ATOM	1142	CA	MET	171	55.555	-3.858	55.434	1.00	25.00
ATOM	1147	C	MET	171	56.946	-4.352	55.011	1.00	25.00
ATOM	1148	O	MET	171	57.949	-3.697	55.287	1.00	25.00
ATOM	1143	CB	MET	171	55.151	-4.471	56.777	1.00	25.00
ATOM	1144	CG	MET	171	55.960	-3.990	57.994	1.00	25.00
ATOM	1145	SD	MET	171	55.705	-2.255	58.485	1.00	25.00
ATOM	1146	CE	MET	171	57.425	-1.813	58.948	1.00	25.00
ATOM	1149	N	GLU	172	56.971	-5.470	54.277	1.00	25.00
ATOM	1150	CA	GLU	172	58.196	-6.085	53.763	1.00	25.00
ATOM	1156	C	GLU	172	58.927	-5.130	52.794	1.00	25.00
ATOM	1157	O	GLU	172	60.173	-5.083	52.772	1.00	25.00
ATOM	1151	CB	GLU	172	57.828	-7.393	53.054	1.00	25.00
ATOM	1152	CG	GLU	172	59.004	-8.369	52.831	1.00	25.00
ATOM	1153	CD	GLU	172	58.652	-9.571	51.929	1.00	25.00
ATOM	1154	OE1	GLU	172	58.299	-9.336	50.736	1.00	25.00
ATOM	1155	OE2	GLU	172	58.754	-10.738	52.415	1.00	25.00
ATOM	1158	N	SER	173	58.122	-4.390	52.009	1.00	25.00
ATOM	1159	CA	SER	173	58.565	-3.369	51.019	1.00	25.00
ATOM	1162	C	SER	173	58.953	-2.072	51.735	1.00	25.00
ATOM	1163	O	SER	173	59.992	-1.471	51.466	1.00	25.00
ATOM	1160	CB	SER	173	57.429	-3.013	50.027	1.00	25.00
ATOM	1161	OG	SER	173	57.335	-3.874	48.903	1.00	25.00
ATOM	1164	N	LYS	174	58.068	-1.616	52.610	1.00	25.00
ATOM	1165	CA	LYS	174	58.311	-0.408	53.351	1.00	25.00
ATOM	1171	C	LYS	174	59.646	-0.578	54.033	1.00	25.00
ATOM	1172	O	LYS	174	60.519	0.265	53.913	1.00	25.00
ATOM	1166	CB	LYS	174	57.186	-0.180	54.355	1.00	25.00
ATOM	1167	CG	LYS	174	55.872	0.145	53.672	1.00	25.00
ATOM	1168	CD	LYS	174	54.867	0.751	54.612	1.00	25.00
ATOM	1169	CE	LYS	174	53.574	1.054	53.890	1.00	25.00
ATOM	1170	NZ	LYS	174	52.441	1.382	54.812	1.00	25.00
ATOM	1173	N	ALA	175	59.850	-1.758	54.600	1.00	25.00
ATOM	1174	CA	ALA	175	61.082	-2.098	55.317	1.00	25.00
ATOM	1176	C	ALA	175	62.319	-1.934	54.472	1.00	25.00
ATOM	1177	O	ALA	175	63.301	-1.311	54.890	1.00	25.00

Fig. 23GG

ATOM	1175	CB	ALA	175	61.012	-3.538	55.810	1.00	25.00
ATOM	1178	N	ARG	176	62.266	-2.559	53.299	1.00	25.00
ATOM	1179	CA	ARG	176	63.356	-2.571	52.339	1.00	25.00
ATOM	1187	C	ARG	176	63.837	-1.185	51.953	1.00	25.00
ATOM	1188	O	ARG	176	65.039	-0.958	51.924	1.00	25.00
ATOM	1180	CB	ARG	176	62.942	-3.385	51.114	1.00	25.00
ATOM	1181	CG	ARG	176	63.987	-3.466	50.042	1.00	25.00
ATOM	1182	CD	ARG	176	65.256	-4.188	50.509	1.00	25.00
ATOM	1183	NE	ARG	176	66.477	-3.772	49.796	1.00	25.00
ATOM	1184	CZ	ARG	176	66.560	-3.460	48.495	1.00	25.00
ATOM	1185	NH1	ARG	176	65.487	-3.492	47.698	1.00	25.00
ATOM	1186	NH2	ARG	176	67.736	-3.099	47.982	1.00	25.00
ATOM	1189	N	LEU	177	62.919	-0.256	51.695	1.00	25.00
ATOM	1190	CA	LEU	177	63.294	1.102	51.321	1.00	25.00
ATOM	1195	C	LEU	177	64.023	1.754	52.476	1.00	25.00
ATOM	1196	O	LEU	177	65.106	2.310	52.323	1.00	25.00
ATOM	1191	CB	LEU	177	62.062	1.941	51.036	1.00	25.00
ATOM	1192	CG	LEU	177	61.005	1.421	50.083	1.00	25.00
ATOM	1193	CD1	LEU	177	59.790	2.281	50.200	1.00	25.00
ATOM	1194	CD2	LEU	177	61.516	1.480	48.694	1.00	25.00
ATOM	1197	N	LEU	178	63.407	1.676	53.647	1.00	25.00
ATOM	1198	CA	LEU	178	63.950	2.264	54.861	1.00	25.00
ATOM	1203	C	LEU	178	65.390	1.855	55.111	1.00	25.00
ATOM	1204	O	LEU	178	66.169	2.644	55.629	1.00	25.00
ATOM	1199	CB	LEU	178	63.067	1.907	56.056	1.00	25.00
ATOM	1200	CG	LEU	178	62.215	3.047	56.623	1.00	25.00
ATOM	1201	CD1	LEU	178	61.738	3.956	55.509	1.00	25.00
ATOM	1202	CD2	LEU	178	61.041	2.493	57.442	1.00	25.00
ATOM	1205	N	SER	179	65.758	0.638	54.732	1.00	25.00
ATOM	1206	CA	SER	179	67.125	0.187	54.938	1.00	25.00
ATOM	1209	C	SER	179	68.056	0.814	53.918	1.00	25.00
ATOM	1210	O	SER	179	69.118	1.343	54.258	1.00	25.00
ATOM	1207	CB	SER	179	67.212	-1.332	54.845	1.00	25.00
ATOM	1208	OG	SER	179	68.571	-1.749	54.923	1.00	25.00
ATOM	1211	N	LEU	180	67.653	0.730	52.658	1.00	25.00
ATOM	1212	CA	LEU	180	68.426	1.291	51.566	1.00	25.00
ATOM	1217	C	LEU	180	68.739	2.728	51.928	1.00	25.00

Fig. 23HH

ATOM	1218	O	LEU	180	69.858	3.183	51.717	1.00	25.00
ATOM	1213	CB	LEU	180	67.628	1.229	50.261	1.00	25.00
ATOM	1214	CG	LEU	180	67.390	-0.184	49.748	1.00	25.00
ATOM	1215	CD1	LEU	180	66.227	-0.205	48.762	1.00	25.00
ATOM	1216	CD2	LEU	180	68.688	-0.692	49.140	1.00	25.00
ATOM	1219	N	VAL	181	67.772	3.409	52.540	1.00	25.00
ATOM	1220	CA	VAL	181	67.956	4.797	52.937	1.00	25.00
ATOM	1224	C	VAL	181	69.083	4.910	53.958	1.00	25.00
ATOM	1225	O	VAL	181	69.940	5.792	53.872	1.00	25.00
ATOM	1221	CB	VAL	181	66.655	5.400	53.517	1.00	25.00
ATOM	1222	CG1	VAL	181	66.863	6.853	53.906	1.00	25.00
ATOM	1223	CG2	VAL	181	65.547	5.283	52.507	1.00	25.00
ATOM	1226	N	LYS	182	69.113	3.982	54.898	1.00	25.00
ATOM	1227	CA	LYS	182	70.139	4.011	55.920	1.00	25.00
ATOM	1233	C	LYS	182	71.538	3.988	55.279	1.00	25.00
ATOM	1234	O	LYS	182	72.459	4.649	55.765	1.00	25.00
ATOM	1228	CB	LYS	182	69.940	2.849	56.897	1.00	25.00
ATOM	1229	CG	LYS	182	70.951	2.818	58.022	1.00	25.00
ATOM	1230	CD	LYS	182	71.073	4.198	58.710	1.00	25.00
ATOM	1231	CE	LYS	182	72.230	4.232	59.754	1.00	25.00
ATOM	1232	NZ	LYS	182	72.420	5.568	60.424	1.00	25.00
ATOM	1235	N	ASP	183	71.700	3.238	54.191	1.00	25.00
ATOM	1236	CA	ASP	183	72.997	3.195	53.525	1.00	25.00
ATOM	1241	C	ASP	183	73.261	4.616	53.073	1.00	25.00
ATOM	1242	O	ASP	183	74.220	5.243	53.507	1.00	25.00
ATOM	1237	CB	ASP	183	72.995	2.339	52.233	1.00	25.00
ATOM	1238	CG	ASP	183	72.736	0.840	52.465	1.00	25.00
ATOM	1239	OD1	ASP	183	72.636	0.362	53.629	1.00	25.00
ATOM	1240	OD2	ASP	183	72.620	0.143	51.425	1.00	25.00
ATOM	1243	N	TYR	184	72.388	5.090	52.182	1.00	25.00
ATOM	1244	CA	TYR	184	72.453	6.415	51.552	1.00	25.00
ATOM	1253	C	TYR	184	73.152	7.519	52.332	1.00	25.00
ATOM	1254	O	TYR	184	72.572	8.134	53.257	1.00	25.00
ATOM	1245	CB	TYR	184	71.043	6.898	51.142	1.00	25.00
ATOM	1246	CG	TYR	184	71.016	8.245	50.439	1.00	25.00
ATOM	1247	CD1	TYR	184	71.331	8.349	49.085	1.00	25.00
ATOM	1249	CD2	TYR	184	70.725	9.418	51.140	1.00	25.00

Fig. 23II

ATOM	1248	CE1	TYR	184	71.368	9.589	48.438	1.00	25.00
ATOM	1250	CE2	TYR	184	70.763	10.665	50.510	1.00	25.00
ATOM	1251	CZ	TYR	184	71.088	10.749	49.153	1.00	25.00
ATOM	1252	OH	TYR	184	71.153	11.983	48.513	1.00	25.00
ATOM	1255	N	ALA	185	74.402	7.771	51.961	1.00	25.00
ATOM	1256	CA	ALA	185	75.141	8.844	52.605	1.00	25.00
ATOM	1258	C	ALA	185	75.074	9.959	51.578	1.00	25.00
ATOM	1259	O	ALA	185	75.139	9.723	50.356	1.00	25.00
ATOM	1257	CB	ALA	185	76.570	8.445	52.903	1.00	25.00
ATOM	1260	N	GLY	186	74.941	11.175	52.083	1.00	25.00
ATOM	1261	CA	GLY	186	74.790	12.311	51.205	1.00	25.00
ATOM	1262	C	GLY	186	73.439	12.907	51.598	1.00	25.00
ATOM	1263	O	GLY	186	72.914	13.826	50.936	1.00	25.00
ATOM	1264	N	LEU	187	72.860	12.416	52.695	1.00	25.00
ATOM	1265	CA	LEU	187	71.589	12.963	53.126	1.00	25.00
ATOM	1270	C	LEU	187	71.814	14.358	53.748	1.00	25.00
ATOM	1271	O	LEU	187	71.018	14.801	54.565	1.00	25.00
ATOM	1266	CB	LEU	187	70.891	12.025	54.108	1.00	25.00
ATOM	1267	CG	LEU	187	71.591	11.897	55.468	1.00	25.00
ATOM	1268	CD1	LEU	187	70.562	11.854	56.601	1.00	25.00
ATOM	1269	CD2	LEU	187	72.544	10.674	55.494	1.00	25.00
ATOM	1272	N	ASN	188	72.919	15.017	53.378	1.00	25.00
ATOM	1273	CA	ASN	188	73.286	16.366	53.858	1.00	25.00
ATOM	1278	C	ASN	188	73.228	17.354	52.662	1.00	25.00
ATOM	1279	O	ASN	188	72.903	18.557	52.814	1.00	25.00
ATOM	1274	CB	ASN	188	74.726	16.360	54.431	1.00	25.00
ATOM	1275	CG	ASN	188	75.625	17.489	53.827	1.00	25.00
ATOM	1276	OD1	ASN	188	76.086	17.397	52.669	1.00	25.00
ATOM	1277	ND2	ASN	188	75.828	18.569	54.600	1.00	25.00
ATOM	1280	N	LYS	189	73.718	16.850	51.531	1.00	25.00
ATOM	1281	CA	LYS	189	73.773	17.542	50.259	1.00	25.00
ATOM	1287	C	LYS	189	72.633	18.551	50.142	1.00	25.00
ATOM	1288	O	LYS	189	71.487	18.144	50.172	1.00	25.00
ATOM	1282	CB	LYS	189	73.562	16.476	49.191	1.00	25.00
ATOM	1283	CG	LYS	189	74.464	16.503	48.014	1.00	25.00
ATOM	1284	CD	LYS	189	74.189	15.256	47.209	1.00	25.00
ATOM	1285	CE	LYS	189	75.188	15.083	46.064	1.00	25.00

Fig. 23JJ

ATOM	1286	NZ	LYS	189	75.394	13.633	45.680	1.00	25.00
ATOM	1289	N	VAL	190	72.909	19.848	50.084	1.00	25.00
ATOM	1290	CA	VAL	190	71.811	20.795	49.911	1.00	25.00
ATOM	1294	C	VAL	190	71.804	21.348	48.467	1.00	25.00
ATOM	1295	O	VAL	190	72.779	21.947	47.997	1.00	25.00
ATOM	1291	CB	VAL	190	71.755	21.929	51.012	1.00	25.00
ATOM	1292	CG1	VAL	190	72.047	21.357	52.390	1.00	25.00
ATOM	1293	CG2	VAL	190	72.671	23.088	50.700	1.00	25.00
ATOM	1296	N	TRP	191	70.746	21.024	47.728	1.00	25.00
ATOM	1297	CA	TRP	191	70.594	21.474	46.355	1.00	25.00
ATOM	1308	C	TRP	191	70.256	22.955	46.296	1.00	25.00
ATOM	1309	O	TRP	191	69.259	23.416	46.853	1.00	25.00
ATOM	1298	CB	TRP	191	69.532	20.642	45.641	1.00	25.00
ATOM	1299	CG	TRP	191	69.995	19.246	45.424	1.00	25.00
ATOM	1303	CD1	TRP	191	70.581	18.741	44.292	1.00	25.00
ATOM	1300	CD2	TRP	191	70.029	18.191	46.396	1.00	25.00
ATOM	1304	NE1	TRP	191	70.995	17.444	44.508	1.00	25.00
ATOM	1301	CE2	TRP	191	70.669	17.082	45.792	1.00	25.00
ATOM	1302	CE3	TRP	191	69.582	18.073	47.717	1.00	25.00
ATOM	1305	CZ2	TRP	191	70.878	15.873	46.474	1.00	25.00
ATOM	1306	CZ3	TRP	191	69.786	16.870	48.391	1.00	25.00
ATOM	1307	CH2	TRP	191	70.429	15.788	47.768	1.00	25.00
ATOM	1310	N	LYS	192	71.130	23.715	45.663	1.00	25.00
ATOM	1311	CA	LYS	192	70.910	25.136	45.542	1.00	25.00
ATOM	1317	C	LYS	192	70.531	25.511	44.128	1.00	25.00
ATOM	1318	O	LYS	192	71.239	25.127	43.183	1.00	25.00
ATOM	1312	CB	LYS	192	72.165	25.896	45.941	1.00	25.00
ATOM	1313	CG	LYS	192	72.369	25.927	47.428	1.00	25.00
ATOM	1314	CD	LYS	192	73.678	26.585	47.794	1.00	25.00
ATOM	1315	CE	LYS	192	73.662	27.012	49.254	1.00	25.00
ATOM	1316	NZ	LYS	192	72.722	28.163	49.484	1.00	25.00
ATOM	1319	N	VAL	193	69.367	26.154	43.974	1.00	25.00
ATOM	1320	CA	VAL	193	68.890	26.660	42.679	1.00	25.00
ATOM	1324	C	VAL	193	68.781	28.139	43.026	1.00	25.00
ATOM	1325	O	VAL	193	69.051	28.515	44.154	1.00	25.00
ATOM	1321	CB	VAL	193	67.522	26.045	42.228	1.00	25.00
ATOM	1322	CG1	VAL	193	67.054	26.695	40.971	1.00	25.00

Fig. 23KK

ATOM	1323	CG2	VAL	193	67.664	24.561	41.939	1.00	25.00
ATOM	1326	N	SER	194	68.374	28.989	42.108	1.00	25.00
ATOM	1327	CA	SER	194	68.339	30.408	42.420	1.00	25.00
ATOM	1330	C	SER	194	66.974	31.056	42.336	1.00	25.00
ATOM	1331	O	SER	194	66.445	31.214	41.250	1.00	25.00
ATOM	1328	CB	SER	194	69.297	31.132	41.476	1.00	25.00
ATOM	1329	OG	SER	194	70.278	30.220	40.973	1.00	25.00
ATOM	1332	N	GLU	195	66.449	31.483	43.478	1.00	25.00
ATOM	1333	CA	GLU	195	65.146	32.147	43.593	1.00	25.00
ATOM	1339	C	GLU	195	64.589	32.746	42.290	1.00	25.00
ATOM	1340	O	GLU	195	63.452	32.453	41.906	1.00	25.00
ATOM	1334	CB	GLU	195	65.235	33.244	44.659	1.00	25.00
ATOM	1335	CG	GLU	195	64.070	33.315	45.618	1.00	25.00
ATOM	1336	CD	GLU	195	64.515	33.550	47.079	1.00	25.00
ATOM	1337	OE1	GLU	195	65.724	33.359	47.386	1.00	25.00
ATOM	1338	OE2	GLU	195	63.651	33.925	47.926	1.00	25.00
ATOM	1341	N	ASP	196	65.410	33.539	41.595	1.00	25.00
ATOM	1342	CA	ASP	196	65.015	34.194	40.343	1.00	25.00
ATOM	1347	C	ASP	196	64.585	33.231	39.259	1.00	25.00
ATOM	1348	O	ASP	196	63.647	33.529	38.538	1.00	25.00
ATOM	1343	CB	ASP	196	66.132	35.106	39.811	1.00	25.00
ATOM	1344	CG	ASP	196	66.162	36.485	40.494	1.00	25.00
ATOM	1345	OD1	ASP	196	65.082	36.924	40.977	1.00	25.00
ATOM	1346	OD2	ASP	196	67.256	37.138	40.525	1.00	25.00
ATOM	1349	N	LYS	197	65.292	32.108	39.120	1.00	25.00
ATOM	1350	CA	LYS	197	64.968	31.070	38.118	1.00	25.00
ATOM	1356	C	LYS	197	63.995	30.021	38.677	1.00	25.00
ATOM	1357	O	LYS	197	63.277	29.329	37.940	1.00	25.00
ATOM	1351	CB	LYS	197	66.232	30.363	37.641	1.00	25.00
ATOM	1352	CG	LYS	197	66.672	29.227	38.512	1.00	25.00
ATOM	1353	CD	LYS	197	66.648	27.962	37.714	1.00	25.00
ATOM	1354	CE	LYS	197	67.537	28.073	36.474	1.00	25.00
ATOM	1355	NZ	LYS	197	68.988	28.283	36.784	1.00	25.00
ATOM	1358	N	LEU	198	63.999	29.909	39.998	1.00	25.00
ATOM	1359	CA	LEU	198	63.142	28.983	40.691	1.00	25.00
ATOM	1364	C	LEU	198	61.737	29.531	40.577	1.00	25.00
ATOM	1365	O	LEU	198	60.817	28.775	40.300	1.00	25.00

Fig. 23LL

ATOM	1360	CB	LEU	198	63.570	28.874	42.150	1.00	25.00
ATOM	1361	CG	LEU	198	63.115	27.632	42.917	1.00	25.00
ATOM	1362	CD1	LEU	198	63.426	26.366	42.127	1.00	25.00
ATOM	1363	CD2	LEU	198	63.788	27.606	44.272	1.00	25.00
ATOM	1366	N	ALA	199	61.590	30.850	40.706	1.00	25.00
ATOM	1367	CA	ALA	199	60.282	31.502	40.617	1.00	25.00
ATOM	1369	C	ALA	199	59.715	31.449	39.199	1.00	25.00
ATOM	1370	O	ALA	199	58.513	31.631	38.983	1.00	25.00
ATOM	1368	CB	ALA	199	60.368	32.923	41.096	1.00	25.00
ATOM	1371	N	LYS	200	60.596	31.170	38.242	1.00	25.00
ATOM	1372	CA	LYS	200	60.223	31.056	36.836	1.00	25.00
ATOM	1378	C	LYS	200	59.851	29.611	36.531	1.00	25.00
ATOM	1379	O	LYS	200	58.930	29.355	35.772	1.00	25.00
ATOM	1373	CB	LYS	200	61.371	31.521	35.915	1.00	25.00
ATOM	1374	CG	LYS	200	61.562	33.045	35.852	1.00	25.00
ATOM	1375	CD	LYS	200	62.792	33.459	35.054	1.00	25.00
ATOM	1376	CE	LYS	200	62.971	35.000	35.082	1.00	25.00
ATOM	1377	NZ	LYS	200	62.095	35.799	34.122	1.00	25.00
ATOM	1380	N	VAL	201	60.574	28.653	37.091	1.00	25.00
ATOM	1381	CA	VAL	201	60.195	27.281	36.824	1.00	25.00
ATOM	1385	C	VAL	201	58.855	27.022	37.518	1.00	25.00
ATOM	1386	O	VAL	201	57.984	26.370	36.963	1.00	25.00
ATOM	1382	CB	VAL	201	61.232	26.253	37.331	1.00	25.00
ATOM	1383	CG1	VAL	201	60.849	24.858	36.858	1.00	25.00
ATOM	1384	CG2	VAL	201	62.617	26.598	36.857	1.00	25.00
ATOM	1387	N	LEU	202	58.686	27.563	38.722	1.00	25.00
ATOM	1388	CA	LEU	202	57.458	27.369	39.490	1.00	25.00
ATOM	1393	C	LEU	202	56.308	28.161	38.909	1.00	25.00
ATOM	1394	O	LEU	202	55.158	27.825	39.138	1.00	25.00
ATOM	1389	CB	LEU	202	57.657	27.690	40.976	1.00	25.00
ATOM	1390	CG	LEU	202	58.604	26.830	41.827	1.00	25.00
ATOM	1391	CD1	LEU	202	58.625	27.356	43.244	1.00	25.00
ATOM	1392	CD2	LEU	202	58.176	25.399	41.833	1.00	25.00
ATOM	1395	N	LEU	203	56.609	29.246	38.205	1.00	25.00
ATOM	1396	CA	LEU	203	55.550	30.001	37.555	1.00	25.00
ATOM	1401	C	LEU	203	55.182	29.199	36.315	1.00	25.00
ATOM	1402	O	LEU	203	54.034	29.165	35.914	1.00	25.00

Fig. 23MM

ATOM	1397	CB	LEU	203	56.015	31.387	37.100	1.00	25.00
ATOM	1398	CG	LEU	203	55.030	32.024	36.105	1.00	25.00
ATOM	1399	CD1	LEU	203	53.795	32.410	36.834	1.00	25.00
ATOM	1400	CD2	LEU	203	55.588	33.219	35.418	1.00	25.00
ATOM	1403	N	SER	204	56.164	28.547	35.704	1.00	25.00
ATOM	1404	CA	SER	204	55.937	27.774	34.486	1.00	25.00
ATOM	1407	C	SER	204	55.042	26.563	34.672	1.00	25.00
ATOM	1408	O	SER	204	54.425	26.109	33.715	1.00	25.00
ATOM	1405	CB	SER	204	57.269	27.352	33.863	1.00	25.00
ATOM	1406	OG	SER	204	57.059	26.597	32.681	1.00	25.00
ATOM	1409	N	THR	205	54.988	26.005	35.877	1.00	25.00
ATOM	1410	CA	THR	205	54.127	24.863	36.064	1.00	25.00
ATOM	1414	C	THR	205	52.680	25.327	36.211	1.00	25.00
ATOM	1415	O	THR	205	51.778	24.578	35.886	1.00	25.00
ATOM	1411	CB	THR	205	54.596	23.900	37.188	1.00	25.00
ATOM	1412	OG1	THR	205	54.474	24.519	38.462	1.00	25.00
ATOM	1413	CG2	THR	205	56.028	23.503	36.980	1.00	25.00
ATOM	1416	N	ALA	206	52.467	26.587	36.601	1.00	25.00
ATOM	1417	CA	ALA	206	51.120	27.164	36.741	1.00	25.00
ATOM	1419	C	ALA	206	50.546	27.503	35.371	1.00	25.00
ATOM	1420	O	ALA	206	49.462	27.055	35.005	1.00	25.00
ATOM	1418	CB	ALA	206	51.155	28.418	37.594	1.00	25.00
ATOM	1421	N	VAL	207	51.280	28.324	34.631	1.00	25.00
ATOM	1422	CA	VAL	207	50.893	28.752	33.295	1.00	25.00
ATOM	1426	C	VAL	207	50.524	27.536	32.443	1.00	25.00
ATOM	1427	O	VAL	207	49.434	27.459	31.887	1.00	25.00
ATOM	1423	CB	VAL	207	52.050	29.547	32.616	1.00	25.00
ATOM	1424	CG1	VAL	207	51.859	29.569	31.111	1.00	25.00
ATOM	1425	CG2	VAL	207	52.111	30.986	33.148	1.00	25.00
ATOM	1428	N	ASN	208	51.422	26.562	32.402	1.00	25.00
ATOM	1429	CA	ASN	208	51.233	25.331	31.648	1.00	25.00
ATOM	1434	C	ASN	208	50.311	24.335	32.296	1.00	25.00
ATOM	1435	O	ASN	208	50.538	23.141	32.160	1.00	25.00
ATOM	1430	CB	ASN	208	52.562	24.637	31.500	1.00	25.00
ATOM	1431	CG	ASN	208	53.429	25.310	30.532	1.00	25.00
ATOM	1432	OD1	ASN	208	53.145	25.306	29.331	1.00	25.00
ATOM	1433	ND2	ASN	208	54.520	25.887	31.015	1.00	25.00

Fig. 23NN

ATOM	1436	N	ASN	209	49.306	24.795	33.033	1.00	25.00
ATOM	1437	CA	ASN	209	48.391	23.884	33.720	1.00	25.00
ATOM	1442	C	ASN	209	47.133	24.601	34.081	1.00	25.00
ATOM	1443	O	ASN	209	46.239	24.031	34.682	1.00	25.00
ATOM	1438	CB	ASN	209	49.025	23.350	35.002	1.00	25.00
ATOM	1439	CG	ASN	209	49.862	22.114	34.768	1.00	25.00
ATOM	1440	OD1	ASN	209	49.322	21.024	34.693	1.00	25.00
ATOM	1441	ND2	ASN	209	51.185	22.271	34.663	1.00	25.00
ATOM	1444	N	MET	210	47.050	25.855	33.685	1.00	25.00
ATOM	1445	CA	MET	210	45.887	26.650	33.996	1.00	25.00
ATOM	1450	C	MET	210	44.580	26.128	33.423	1.00	25.00
ATOM	1451	O	MET	210	43.536	26.277	34.039	1.00	25.00
ATOM	1446	CB	MET	210	46.110	28.084	33.542	1.00	25.00
ATOM	1447	CG	MET	210	46.471	28.212	32.099	1.00	25.00
ATOM	1448	SD	MET	210	46.890	29.872	31.686	1.00	25.00
ATOM	1449	CE	MET	210	46.941	29.769	29.920	1.00	25.00
ATOM	1452	N	LEU	211	44.643	25.484	32.265	1.00	25.00
ATOM	1453	CA	LEU	211	43.442	24.994	31.595	1.00	25.00
ATOM	1458	C	LEU	211	42.882	23.673	32.079	1.00	25.00
ATOM	1459	O	LEU	211	41.719	23.388	31.837	1.00	25.00
ATOM	1454	CB	LEU	211	43.651	24.963	30.077	1.00	25.00
ATOM	1455	CG	LEU	211	43.678	26.229	29.197	1.00	25.00
ATOM	1456	CD1	LEU	211	43.898	27.517	29.960	1.00	25.00
ATOM	1457	CD2	LEU	211	44.750	26.034	28.162	1.00	25.00
ATOM	1460	N	LEU	212	43.691	22.885	32.777	1.00	25.00
ATOM	1461	CA	LEU	212	43.271	21.585	33.321	1.00	25.00
ATOM	1466	C	LEU	212	42.067	21.675	34.274	1.00	25.00
ATOM	1467	O	LEU	212	42.030	22.500	35.187	1.00	25.00
ATOM	1462	CB	LEU	212	44.479	20.902	33.980	1.00	25.00
ATOM	1463	CG	LEU	212	44.459	20.006	35.214	1.00	25.00
ATOM	1464	CD1	LEU	212	43.726	18.699	35.006	1.00	25.00
ATOM	1465	CD2	LEU	212	45.900	19.739	35.587	1.00	25.00
ATOM	1468	N	ARG	213	41.059	20.845	34.035	1.00	25.00
ATOM	1469	CA	ARG	213	39.862	20.849	34.867	1.00	25.00
ATOM	1477	C	ARG	213	39.782	19.676	35.834	1.00	25.00
ATOM	1478	O	ARG	213	40.389	18.630	35.609	1.00	25.00
ATOM	1470	CB	ARG	213	38.622	20.947	33.994	1.00	25.00

Fig. 2300

ATOM	1471	CG	ARG	213	38.243	22.385	33.746	1.00	25.00
ATOM	1472	CD	ARG	213	37.771	22.613	32.343	1.00	25.00
ATOM	1473	NE	ARG	213	38.569	23.631	31.672	1.00	25.00
ATOM	1474	CZ	ARG	213	38.052	24.720	31.128	1.00	25.00
ATOM	1475	NH1	ARG	213	36.740	24.922	31.213	1.00	25.00
ATOM	1476	NH2	ARG	213	38.836	25.605	30.523	1.00	25.00
ATOM	1479	N	ASP	214	39.014	19.851	36.907	1.00	25.00
ATOM	1480	CA	ASP	214	38.893	18.842	37.959	1.00	25.00
ATOM	1485	C	ASP	214	40.295	18.416	38.407	1.00	25.00
ATOM	1486	O	ASP	214	40.599	17.238	38.583	1.00	25.00
ATOM	1481	CB	ASP	214	38.049	17.656	37.507	1.00	25.00
ATOM	1482	CG	ASP	214	36.612	18.046	37.203	1.00	25.00
ATOM	1483	OD1	ASP	214	36.101	19.028	37.797	1.00	25.00
ATOM	1484	OD2	ASP	214	35.997	17.357	36.358	1.00	25.00
ATOM	1487	N	ARG	215	41.133	19.431	38.587	1.00	25.00
ATOM	1488	CA	ARG	215	42.510	19.319	39.022	1.00	25.00
ATOM	1496	C	ARG	215	42.571	18.475	40.288	1.00	25.00
ATOM	1497	O	ARG	215	43.172	17.410	40.302	1.00	25.00
ATOM	1489	CB	ARG	215	42.996	20.731	39.298	1.00	25.00
ATOM	1490	CG	ARG	215	44.391	20.905	39.829	1.00	25.00
ATOM	1491	CD	ARG	215	44.606	22.396	40.184	1.00	25.00
ATOM	1492	NE	ARG	215	43.882	23.226	39.230	1.00	25.00
ATOM	1493	CZ	ARG	215	44.437	23.871	38.214	1.00	25.00
ATOM	1494	NH1	ARG	215	45.759	23.891	38.093	1.00	25.00
ATOM	1495	NH2	ARG	215	43.672	24.573	37.378	1.00	25.00
ATOM	1498	N	TRP	216	41.874	18.921	41.326	1.00	25.00
ATOM	1499	CA	TRP	216	41.868	18.219	42.599	1.00	25.00
ATOM	1510	C	TRP	216	41.113	16.934	42.574	1.00	25.00
ATOM	1511	O	TRP	216	41.299	16.124	43.472	1.00	25.00
ATOM	1500	CB	TRP	216	41.374	19.105	43.745	1.00	25.00
ATOM	1501	CG	TRP	216	42.306	20.248	44.009	1.00	25.00
ATOM	1505	CD1	TRP	216	42.074	21.565	43.749	1.00	25.00
ATOM	1502	CD2	TRP	216	43.679	20.152	44.383	1.00	25.00
ATOM	1506	NE1	TRP	216	43.225	22.287	43.898	1.00	25.00
ATOM	1503	CE2	TRP	216	44.228	21.447	44.286	1.00	25.00
ATOM	1504	CE3	TRP	216	44.503	19.093	44.765	1.00	25.00
ATOM	1507	CZ2	TRP	216	45.559	21.716	44.548	1.00	25.00

Fig. 23PP

ATOM	1508	CZ3	TRP	216	45.820	19.350	45.025	1.00	25.00
ATOM	1509	CH2	TRP	216	46.344	20.664	44.913	1.00	25.00
ATOM	1512	N	ASP	217	40.267	16.734	41.563	1.00	25.00
ATOM	1513	CA	ASP	217	39.507	15.482	41.445	1.00	25.00
ATOM	1518	C	ASP	217	40.412	14.451	40.796	1.00	25.00
ATOM	1519	O	ASP	217	40.354	13.274	41.112	1.00	25.00
ATOM	1514	CB	ASP	217	38.239	15.658	40.614	1.00	25.00
ATOM	1515	CG	ASP	217	37.207	16.561	41.286	1.00	25.00
ATOM	1516	OD1	ASP	217	37.026	16.476	42.531	1.00	25.00
ATOM	1517	OD2	ASP	217	36.561	17.359	40.552	1.00	25.00
ATOM	1520	N	VAL	218	41.242	14.909	39.873	1.00	25.00
ATOM	1521	CA	VAL	218	42.196	14.052	39.213	1.00	25.00
ATOM	1525	C	VAL	218	43.137	13.603	40.314	1.00	25.00
ATOM	1526	O	VAL	218	43.286	12.425	40.540	1.00	25.00
ATOM	1522	CB	VAL	218	42.970	14.829	38.177	1.00	25.00
ATOM	1523	CG1	VAL	218	44.153	14.024	37.699	1.00	25.00
ATOM	1524	CG2	VAL	218	42.051	15.213	37.050	1.00	25.00
ATOM	1527	N	VAL	219	43.728	14.551	41.033	1.00	25.00
ATOM	1528	CA	VAL	219	44.621	14.229	42.134	1.00	25.00
ATOM	1532	C	VAL	219	43.884	13.449	43.216	1.00	25.00
ATOM	1533	O	VAL	219	44.493	12.723	43.993	1.00	25.00
ATOM	1529	CB	VAL	219	45.229	15.476	42.734	1.00	25.00
ATOM	1530	CG1	VAL	219	46.113	15.143	43.886	1.00	25.00
ATOM	1531	CG2	VAL	219	46.026	16.162	41.692	1.00	25.00
ATOM	1534	N	ALA	220	42.570	13.577	43.279	1.00	25.00
ATOM	1535	CA	ALA	220	41.827	12.821	44.270	1.00	25.00
ATOM	1537	C	ALA	220	41.940	11.350	43.921	1.00	25.00
ATOM	1538	O	ALA	220	42.381	10.566	44.735	1.00	25.00
ATOM	1536	CB	ALA	220	40.383	13.237	44.284	1.00	25.00
ATOM	1539	N	LYS	221	41.614	10.986	42.684	1.00	25.00
ATOM	1540	CA	LYS	221	41.667	9.584	42.290	1.00	25.00
ATOM	1546	C	LYS	221	43.048	8.963	42.085	1.00	25.00
ATOM	1547	O	LYS	221	43.196	7.761	42.328	1.00	25.00
ATOM	1541	CB	LYS	221	40.717	9.270	41.125	1.00	25.00
ATOM	1542	CG	LYS	221	41.118	9.824	39.784	1.00	25.00
ATOM	1543	CD	LYS	221	39.919	9.985	38.844	1.00	25.00
ATOM	1544	CE	LYS	221	39.059	11.207	39.242	1.00	25.00

Fig. 23QQ

ATOM	1545	NZ	LYS	221	38.729	11.325	40.729	1.00	25.00
ATOM	1548	N	ARG	222	44.055	9.746	41.675	1.00	25.00
ATOM	1549	CA	ARG	222	45.412	9.211	41.496	1.00	25.00
ATOM	1557	C	ARG	222	45.899	8.813	42.887	1.00	25.00
ATOM	1558	O	ARG	222	46.632	7.831	43.048	1.00	25.00
ATOM	1550	CB	ARG	222	46.358	10.270	40.953	1.00	25.00
ATOM	1551	CG	ARG	222	45.981	10.892	39.618	1.00	25.00
ATOM	1552	CD	ARG	222	46.301	9.960	38.477	1.00	25.00
ATOM	1553	NE	ARG	222	46.291	10.609	37.163	1.00	25.00
ATOM	1554	CZ	ARG	222	47.148	11.553	36.764	1.00	25.00
ATOM	1555	NH1	ARG	222	48.091	12.037	37.577	1.00	25.00
ATOM	1556	NH2	ARG	222	47.034	12.039	35.538	1.00	25.00
ATOM	1559	N	ARG	223	45.470	9.586	43.889	1.00	25.00
ATOM	1560	CA	ARG	223	45.803	9.369	45.298	1.00	25.00
ATOM	1568	C	ARG	223	45.230	8.020	45.757	1.00	25.00
ATOM	1569	O	ARG	223	45.943	7.192	46.313	1.00	25.00
ATOM	1561	CB	ARG	223	45.200	10.495	46.131	1.00	25.00
ATOM	1562	CG	ARG	223	45.998	10.938	47.352	1.00	25.00
ATOM	1563	CD	ARG	223	45.149	11.867	48.240	1.00	25.00
ATOM	1564	NE	ARG	223	43.906	11.195	48.605	1.00	25.00
ATOM	1565	CZ	ARG	223	43.747	10.453	49.699	1.00	25.00
ATOM	1566	NH1	ARG	223	44.708	10.376	50.622	1.00	25.00
ATOM	1567	NH2	ARG	223	42.588	9.846	49.913	1.00	25.00
ATOM	1570	N	ARG	224	43.945	7.799	45.501	1.00	25.00
ATOM	1571	CA	ARG	224	43.277	6.559	45.853	1.00	25.00
ATOM	1579	C	ARG	224	43.915	5.375	45.132	1.00	25.00
ATOM	1580	O	ARG	224	43.977	4.273	45.653	1.00	25.00
ATOM	1572	CB	ARG	224	41.813	6.655	45.459	1.00	25.00
ATOM	1573	CG	ARG	224	40.861	6.799	46.602	1.00	25.00
ATOM	1574	CD	ARG	224	40.657	5.468	47.308	1.00	25.00
ATOM	1575	NE	ARG	224	39.246	5.047	47.347	1.00	25.00
ATOM	1576	CZ	ARG	224	38.295	5.622	48.092	1.00	25.00
ATOM	1577	NH1	ARG	224	38.575	6.655	48.892	1.00	25.00
ATOM	1578	NH2	ARG	224	37.054	5.151	48.042	1.00	25.00
ATOM	1581	N	GLU	225	44.365	5.589	43.908	1.00	25.00
ATOM	1582	CA	GLU	225	44.987	4.508	43.165	1.00	25.00
ATOM	1588	C	GLU	225	46.335	4.132	43.780	1.00	25.00

Fig. 23RR

ATOM	1589	O	GLU	225	46.682	2.954	43.841	1.00	25.00
ATOM	1583	CB	GLU	225	45.147	4.853	41.656	1.00	25.00
ATOM	1584	CG	GLU	225	44.012	4.373	40.698	1.00	25.00
ATOM	1585	CD	GLU	225	43.690	2.833	40.763	1.00	25.00
ATOM	1586	OE1	GLU	225	44.349	2.063	41.502	1.00	25.00
ATOM	1587	OE2	GLU	225	42.749	2.378	40.066	1.00	25.00
ATOM	1590	N	ALA	226	47.089	5.112	44.264	1.00	25.00
ATOM	1591	CA	ALA	226	48.395	4.799	44.845	1.00	25.00
ATOM	1593	C	ALA	226	48.293	4.076	46.189	1.00	25.00
ATOM	1594	O	ALA	226	49.260	3.483	46.677	1.00	25.00
ATOM	1592	CB	ALA	226	49.239	6.062	44.982	1.00	25.00
ATOM	1595	N	GLY	227	47.112	4.074	46.779	1.00	25.00
ATOM	1596	CA	GLY	227	46.983	3.425	48.061	1.00	25.00
ATOM	1597	C	GLY	227	47.088	4.454	49.167	1.00	25.00
ATOM	1598	O	GLY	227	47.102	4.087	50.343	1.00	25.00
ATOM	1599	N	ILE	228	47.214	5.734	48.811	1.00	25.00
ATOM	1600	CA	ILE	228	47.280	6.779	49.819	1.00	25.00
ATOM	1605	C	ILE	228	45.832	6.950	50.224	1.00	25.00
ATOM	1606	O	ILE	228	45.099	7.744	49.656	1.00	25.00
ATOM	1601	CB	ILE	228	47.791	8.118	49.266	1.00	25.00
ATOM	1603	CG1	ILE	228	49.182	7.974	48.642	1.00	25.00
ATOM	1602	CG2	ILE	228	47.840	9.137	50.376	1.00	25.00
ATOM	1604	CD1	ILE	228	49.816	9.318	48.208	1.00	25.00
ATOM	1607	N	MET	229	45.390	6.099	51.128	1.00	25.00
ATOM	1608	CA	MET	229	44.012	6.157	51.597	1.00	25.00
ATOM	1613	C	MET	229	44.018	6.987	52.879	1.00	25.00
ATOM	1614	O	MET	229	43.072	7.746	53.142	1.00	25.00
ATOM	1609	CB	MET	229	43.486	4.727	51.839	1.00	25.00
ATOM	1610	CG	MET	229	42.031	4.457	51.474	1.00	25.00
ATOM	1611	SD	MET	229	40.858	4.995	52.693	1.00	25.00
ATOM	1612	CE	MET	229	40.597	6.691	52.168	1.00	25.00
ATOM	1615	N	GLY	230	45.147	6.898	53.596	1.00	25.00
ATOM	1616	CA	GLY	230	45.361	7.613	54.854	1.00	25.00
ATOM	1617	C	GLY	230	44.331	8.616	55.401	1.00	25.00
ATOM	1618	O	GLY	230	44.402	9.817	55.066	1.00	25.00
ATOM	1619	N	ALA	231	43.426	8.105	56.260	1.00	25.00

Fig. 23SS

ATOM	1620	CA	ALA	231	42.335	8.836	56.938	1.00	25.00
ATOM	1622	C	ALA	231	41.172	7.899	57.268	1.00	25.00
ATOM	1623	O	ALA	231	40.438	7.572	56.296	1.00	25.00
ATOM	1621	CB	ALA	231	41.811	9.977	56.088	1.00	25.00
ATOM	1624	OT	ALA	231	40.983	7.537	58.470	1.00	25.00

Fig. 24A

Distances that are less than 5Å for residues near active site

52N	139CE1	D = 4.485
52CA	139CE1	D = 3.322
52CA	139ND1	D = 4.089
52CA	139NE2	D = 4.278
52C	54N	D = 3.582
52C	52CG	D = 3.843
52C	139CE1	D = 3.925
52C	139ND1	D = 4.575
52C	52ND1	D = 4.589
52C	139NE2	D = 4.735
52C	54CA	D = 4.789

52O	54N	D = 3.154
52O	139CE1	D = 3.836
52O	54CG	D = 4.074
52O	54CA	D = 4.248
52O	139NE2	D = 4.344
52O	139ND1	D = 4.579
52O	54CB	D = 4.743
52CB	139CE1	D = 3.493
52CB	139NE2	D = 4.071
52CB	139ND1	D = 4.606
52CG	139CE1	D = 3.505
52CG	139NE2	D = 4.012
52CG	122OG	D = 4.202
52CG	139ND1	D = 4.620
52ND1	139CE1	D = 2.831
52ND1	122OG	D = 2.845
52ND1	139NE2	D = 3.146
52ND1	122CB	D = 3.770
52ND1	139ND1	D = 3.919
52ND1	139CD2	D = 4.346
52ND1	120O	D = 4.646
52ND1	139CG	D = 4.735
52ND1	122CA	D = 4.785
52ND1	122N	D = 4.876
52ND1	120CB	D = 4.916
52CD2	120CB	D = 4.632
52CD2	139CE1	D = 4.723
52CD2	120OG	D = 4.867
52CD2	122OG	D = 4.892
52CE1	122OG	D = 2.995
52CE1	120CB	D = 3.738
52CE1	122CB	D = 3.776
52CE1	120O	D = 3.897
52CE1	139CE1	D = 3.939
52CE1	120OG	D = 4.013

Fig. 24B

52CE1 139NE2	D = 4.167
52CE1 122N	D = 4.323
52CE1 122CA	D = 4.387
52CE1 120C	D = 4.402
52CE1 120CA	D = 4.732
52CE1 139ND1	D = 4.855
52NE2 120CB	D = 3.469
52NE2 120OG	D = 3.590
52NE2 122OG	D = 4.313
52NE2 120O	D = 4.549
52NE2 120CA	D = 4.774
52NE2 120C	D = 4.859
52NE2 139CE1	D = 4.952
120N 143SG	D = 4.206
120CA 143SG	D = 4.775
120CA 122N	D = 4.929
120C 122N	D = 3.578
120C 139O	D = 4.571
120C 122OG	D = 4.742
120C 122CA	D = 4.829
120O 122N	D = 3.321
120O 139O	D = 3.665
120O 122OG	D = 3.957
120O 139C	D = 4.344
120O 122CA	D = 4.562
120O 122CB	D = 4.878
120CB 143SG	D = 4.159
120OG 147CG	D = 4.135
120OG 147N	D = 4.695
120OG 143SG	D = 4.755
120OG 147CD	D = 4.956
122N 139O	D = 2.869
122N 139C	D = 4.101
122N 139N	D = 4.893
122N 139CD2	D = 4.976
122CA 139O	D = 3.654
122CA 139NE2	D = 4.662
122CA 139CD2	D = 4.707
122CA 139C	D = 4.854
122C 139O	D = 4.005
122C 139N	D = 4.677
122O 139N	D = 3.662
122O 139O	D = 3.689
122O 139CD2	D = 4.560
122O 139C	D = 4.599
122O 139CA	D = 4.710

Fig. 24C

122CB 139NE2	D = 3.226
122CB 139CD2	D = 3.445
122CB 139O	D = 3.567
122CB 139CE1	D = 4.066
122CB 139CG	D = 4.367
122CB 139C	D = 4.599
122CB 139N	D = 4.645
122CB 139ND1	D = 4.681

122OG 139NE2	D = 2.502
122OG 139O	D = 2.845
122OG 139CD2	D = 2.869
122OG 139CE1	D = 2.957
122OG 139CG	D = 3.470
122OG 139ND1	D = 3.505
122OG 139C	D = 3.751
122OG 139N	D = 4.414
122OG 139CA	D = 4.428
122OG 139CB	D = 4.536

147N 148N	D = 2.763
147N 148CA	D = 4.206
147N 148O	D = 4.648
147N 148C	D = 4.921
147N 148CB	D = 4.983
147CA 148N	D = 2.467
147CA 148CA	D = 3.866
147CA 148C	D = 4.737
147CA 148O	D = 4.751
147CA 148CB	D = 4.833
147CA 148CG	D = 4.968
147C 148N	D = 1.346
147C 148CA	D = 2.481
147C 148C	D = 3.368
147C 148O	D = 3.633
147C 148CB	D = 3.661

147C 147CG	D = 3.767
147C 148CG	D = 3.935
147C 147CD	D = 4.818
147O 148N	D = 2.274
147O 148CA	D = 2.838
147O 148C	D = 3.507
147O 148O	D = 3.945
147O 148CB	D = 4.172
147O 148CG	D = 4.365
147CB 148N	D = 3.207
147CB 148CA	D = 4.516
147CB 148CG	D = 4.846
147CG 148N	D = 4.211

Fig. 25A

Angles of Atoms that are 4.0 Å or less apart (Triad Atoms Only)

52N	52CA	139CE1	A = 134.31
52CB	52CA	139CE1	A = 83.36
52C	52CA	139CE1	A = 101.41
52O	52CA	139CE1	A = 82.46
52CG	52CA	139CE1	A = 72.11
139CE1	52CA	52ND1	A = 50.37
139CE1	52CA	52CD2	A = 86.90
52O	52C	139CE1	A = 76.83
52CA	52C	139CE1	A = 56.07
52N	52C	139CE1	A = 85.67
52CB	52C	139CE1	A = 61.20
52CG	52C	139CE1	A = 53.63
52C	52O	139CE1	A = 85.04
52CA	52O	139CE1	A = 59.15
52CB	52O	139CE1	A = 60.95
52N	52O	139CE1	A = 73.85
52CG	52CB	139CE1	A = 78.17
52CA	52CB	139CE1	A = 70.88
52C	52CB	139CE1	A = 79.99
52N	52CB	139CE1	A = 95.17
52ND1	52CB	139CE1	A = 53.19
52CD2	52CB	139CE1	A = 101.02
52O	52CB	139CE1	A = 73.78
52CD2	52CG	139CE1	A = 149.37
52ND1	52CG	139CE1	A = 50.27
52CB	52CG	139CE1	A = 77.24
52CE1	52CG	139CE1	A = 84.02
52NE2	52CG	139CE1	A = 116.99
52CA	52CG	139CE1	A = 64.42
52N	52CG	139CE1	A = 84.83
139CE1	52CG	52C	A = 64.38
52CE1	52ND1	139CE1	A = 138.45
52CE1	52ND1	139NE2	A = 132.02
52CE1	52ND1	139ND1	A = 127.47
52CG	52ND1	139CE1	A = 107.81
52CG	52ND1	139NE2	A = 119.91
52CG	52ND1	139ND1	A = 112.35
52CD2	52ND1	139CE1	A = 141.02
52CD2	52ND1	139NE2	A = 156.82
52CD2	52ND1	139ND1	A = 139.71
52NE2	52ND1	139CE1	A = 159.45
52NE2	52ND1	139NE2	A = 165.85

Fig. 25B

52NE2	52ND1	139ND1	A =146.98
52CB	52ND1	139CE1	A = 81.02
52CB	52ND1	139NE2	A = 90.90
52CB	52ND1	139ND1	A = 88.36
139CE1	52ND1	139NE2	A = 24.69
139CE1	52ND1	52CA	A = 64.66
139CE1	52ND1	139ND1	A = 12.99
139NE2	52ND1	52CA	A = 82.63
139NE2	52ND1	139ND1	A = 33.57
52CA	52ND1	139ND1	A = 68.12
52NE2	52CE1	120CB	A = 68.06
52NE2	52CE1	1200	A =111.47
52NE2	52CE1	139CE1	A =134.35
52ND1	52CE1	120CB	A =146.58
52ND1	52CE1	1200	A =115.99
52ND1	52CE1	139CE1	A = 28.47
52CD2	52CE1	120CB	A =100.18
52CD2	52CE1	1200	A =132.01
52CD2	52CE1	139CE1	A = 97.30
52CG	52CE1	120CB	A =128.86
52CG	52CE1	1200	A =133.49
52CG	52CE1	139CE1	A = 62.25
52CB	52CE1	120CB	A =134.87
52CB	52CE1	1200	A =131.47
52CB	52CE1	139CE1	A = 54.74
120CB	52CE1	1200	A = 45.13
120CB	52CE1	139CE1	A =128.87
1200	52CE1	139CE1	A = 88.92
52CE1	52NE2	120CB	A = 91.28
52CE1	52NE2	120OG	A = 98.93
52CD2	52NE2	120CB	A =140.77
52CD2	52NE2	120OG	A =152.33
52ND1	52NE2	120CB	A =118.56
52ND1	52NE2	120OG	A =132.30
52CG	52NE2	120CB	A =140.35
52CG	52NE2	120OG	A =162.95
120CB	52NE2	120OG	A = 23.31
120C	1200	1390	A =132.85
120C	1200	52CE1	A =106.93
120CA	1200	1390	A =166.12
120CA	1200	52CE1	A = 95.13
120N	1200	1390	A =158.93
120N	1200	52CE1	A =109.96
120CB	1200	1390	A =150.80
120CB	1200	52CE1	A = 64.57
1390	1200	52CE1	A = 87.10
1390	1200	120OG	A =139.73
52CE1	1200	120OG	A = 61.60
120OG	120CB	52NE2	A = 83.13
120OG	120CB	52CE1	A = 90.41
120CA	120CB	52NE2	A =142.75

Fig. 25C

120CA	120CB	52CE1	A =122.20
120N	120CB	52NE2	A =141.26
120N	120CB	52CE1	A =129.22
120C	120CB	52NE2	A =108.31
120C	120CB	52CE1	A = 87.65
120O	120CB	52NE2	A = 90.15
120O	120CB	52CE1	A = 70.30
52NE2	120CB	52CE1	A = 20.66
120CB	120OG	52NE2	A = 73.56
120CA	120OG	52NE2	A =102.89
120C	120OG	52NE2	A = 89.93
139CG	139O	120O	A =115.86
139CB	139O	120O	A =131.13
139CD2	139O	120O	A =116.26
120O	139O	139ND1	A = 95.03
139CG	139ND1	52ND1	A =118.70
139NE2	139ND1	52ND1	A = 53.28
139CD2	139ND1	52ND1	A = 85.97
139CB	139ND1	52ND1	A =140.80
139C	139ND1	52ND1	A =102.41
139CA	139ND1	52ND1	A =121.31
139O	139ND1	52ND1	A = 84.59
139NE2	139CE1	52ND1	A = 91.17
139NE2	139CE1	52CA	A =129.33
139NE2	139CE1	52CB	A =106.74
139NE2	139CE1	52CG	A =103.06
139NE2	139CE1	52O	A =103.92
139NE2	139CE1	52C	A =120.82
139NE2	139CE1	52CE1	A = 90.65
139ND1	139CE1	52ND1	A =138.26
139ND1	139CE1	52CA	A =116.59
139ND1	139CE1	52CB	A =141.80
139ND1	139CE1	52CG	A =141.97
139ND1	139CE1	52O	A =116.29
139ND1	139CE1	52C	A =111.31
139ND1	139CE1	52CE1	A =127.21
139CD2	139CE1	52ND1	A =120.63
139CD2	139CE1	52CA	A =160.30
139CD2	139CE1	52CB	A =144.04
139CD2	139CE1	52CG	A =138.33
139CD2	139CE1	52O	A =122.44
139CD2	139CE1	52C	A =139.65
139CD2	139CE1	52CE1	A =114.05
139CG	139CE1	52ND1	A =141.07
139CG	139CE1	52CA	A =150.05
139CG	139CE1	52CB	A =173.03
139CG	139CE1	52CG	A =162.38
139CG	139CE1	52O	A =127.77
139CG	139CE1	52C	A =134.72
139CG	139CE1	52CE1	A =128.75
52ND1	139CE1	52CA	A = 64.97

Fig. 25D

52ND1	139CE1	52CB	A = 45.79
52ND1	139CE1	52CG	A = 21.92
52ND1	139CE1	139CB	A = 141.56
52ND1	139CE1	52O	A = 90.42
52ND1	139CE1	52C	A = 83.89
52ND1	139CE1	52CE1	A = 13.08
52CA	139CE1	52CB	A = 25.76
52CA	139CE1	52CG	A = 43.47
52CA	139CE1	139CB	A = 143.49
52CA	139CE1	52O	A = 38.38
52CA	139CE1	52C	A = 22.52
52CA	139CE1	52CE1	A = 75.02
52CB	139CE1	52CG	A = 24.59
52CB	139CE1	139CB	A = 169.20
52CB	139CE1	52O	A = 45.27
52CB	139CE1	52C	A = 38.80
52CB	139CE1	52CE1	A = 58.19
52CG	139CE1	139CB	A = 160.08
52CG	139CE1	52O	A = 69.85
52CG	139CE1	52C	A = 61.99
52CG	139CE1	52CE1	A = 33.73
139CB	139CE1	52O	A = 127.95
139CB	139CE1	52C	A = 131.56
139CB	139CE1	52CE1	A = 128.59
52O	139CE1	52C	A = 18.13
52O	139CE1	52CE1	A = 103.22
52C	139CE1	52CE1	A = 95.37
139CE1	139NE2	52ND1	A = 64.13
139CD2	139NE2	52ND1	A = 144.94
139ND1	139NE2	52ND1	A = 93.14
139CG	139NE2	52ND1	A = 122.96
52ND1	139NE2	139CB	A = 126.15

Fig. 26

	Phi $C_n-1-N_n-C_{An}-C$	Psi $N-CA-C-N_{n+1}$	Omega 1 $CA_n-1-C_n-1-N_n-CA_n$	Omega 2 $CA_n-C_n-N_{n+1}-CA_{n+1}$	Chi1 $N-CA-CB-CG$	Chi2 $CA-CD-CG-XD$
Ser120	120	-120	118	-179	-180	-141
His52	71	13	-178	179	-69	-81
His139	-158	155	178	180	74	111

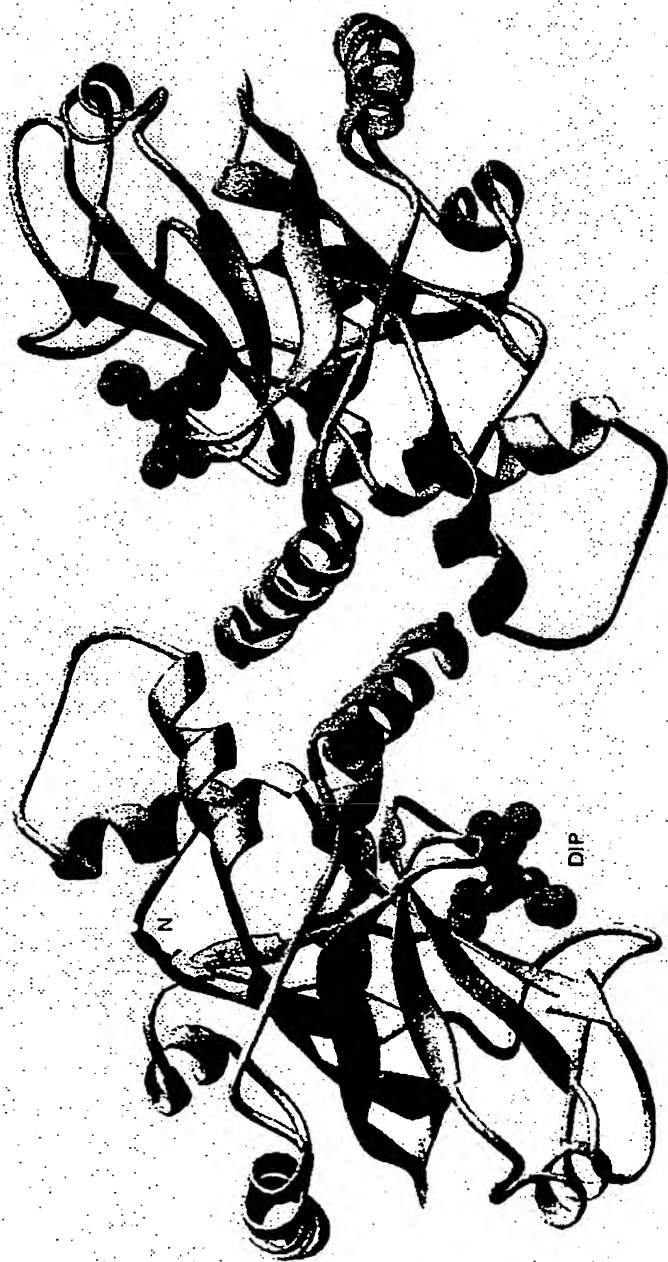


Fig. 27A

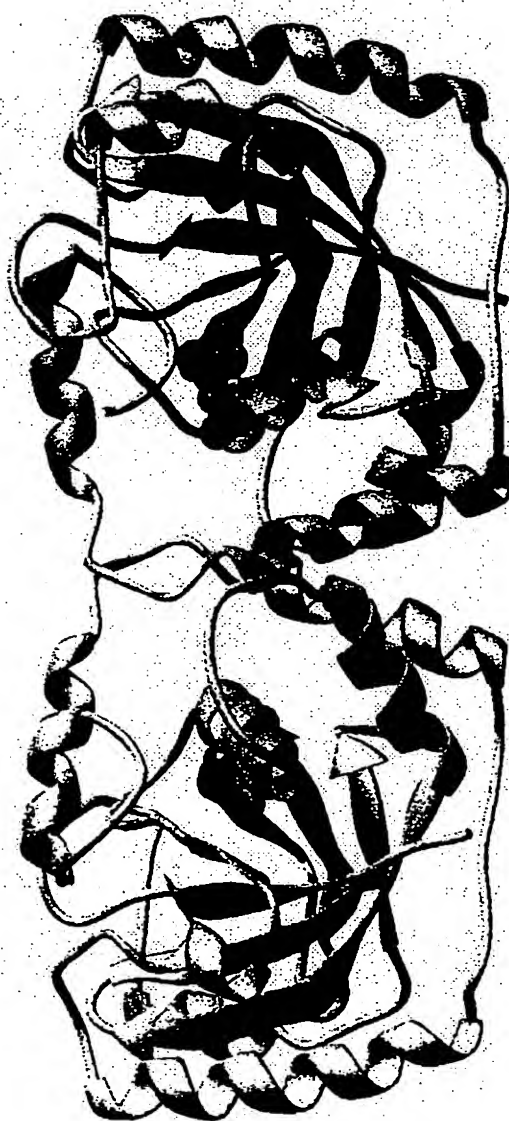


Fig. 2/B

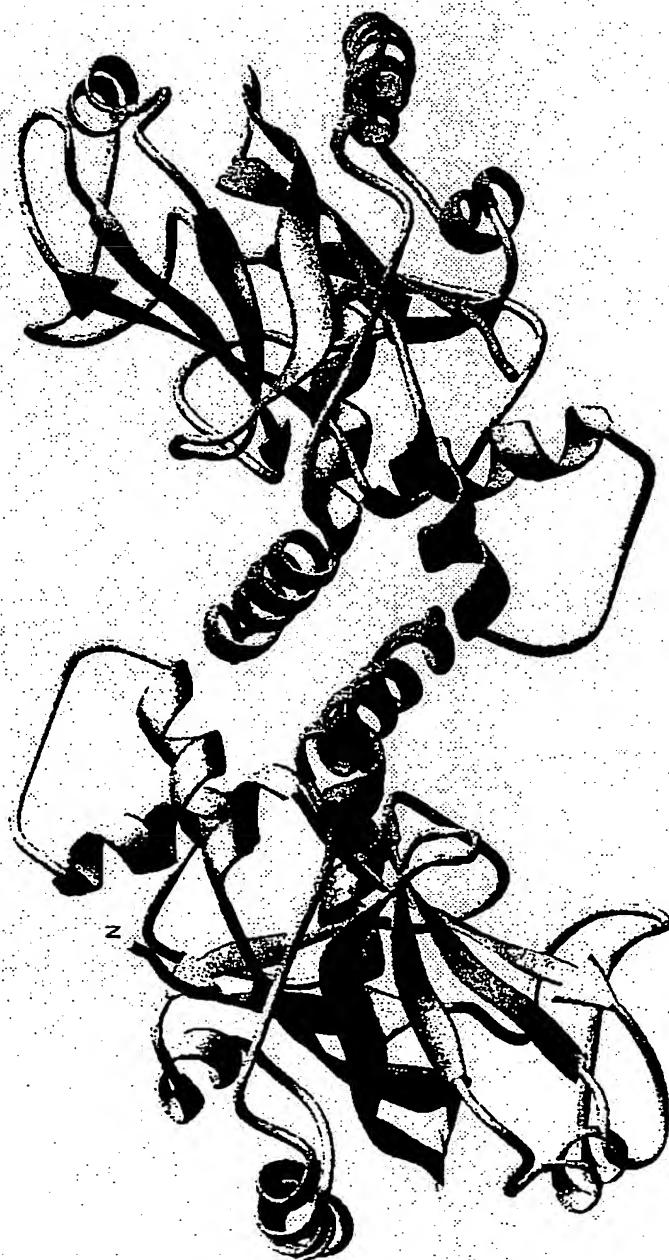


Fig. 27C

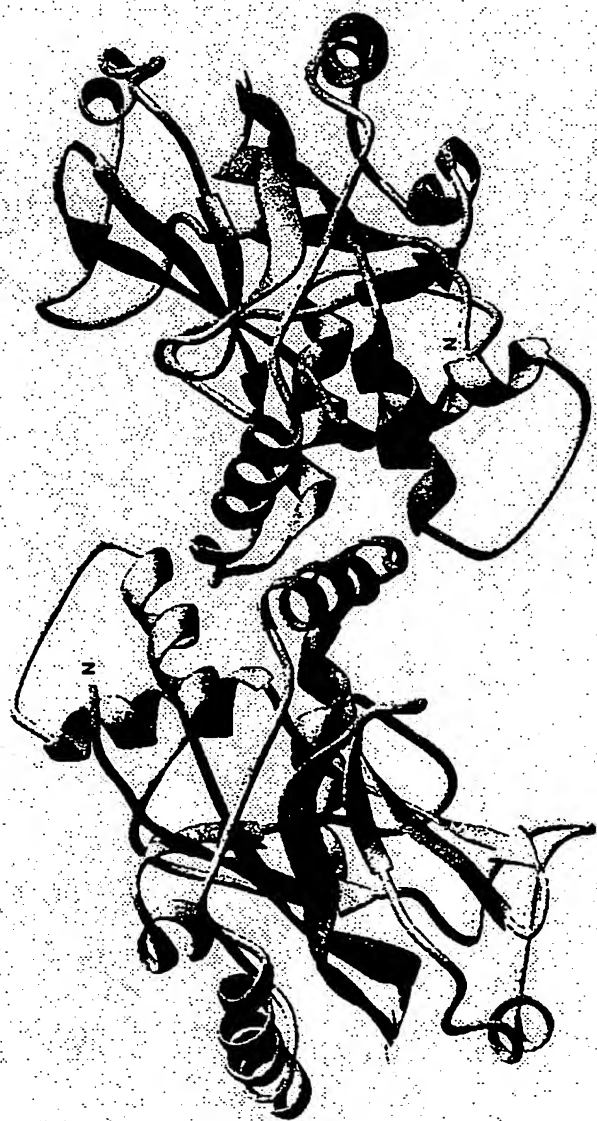


Fig. 28A

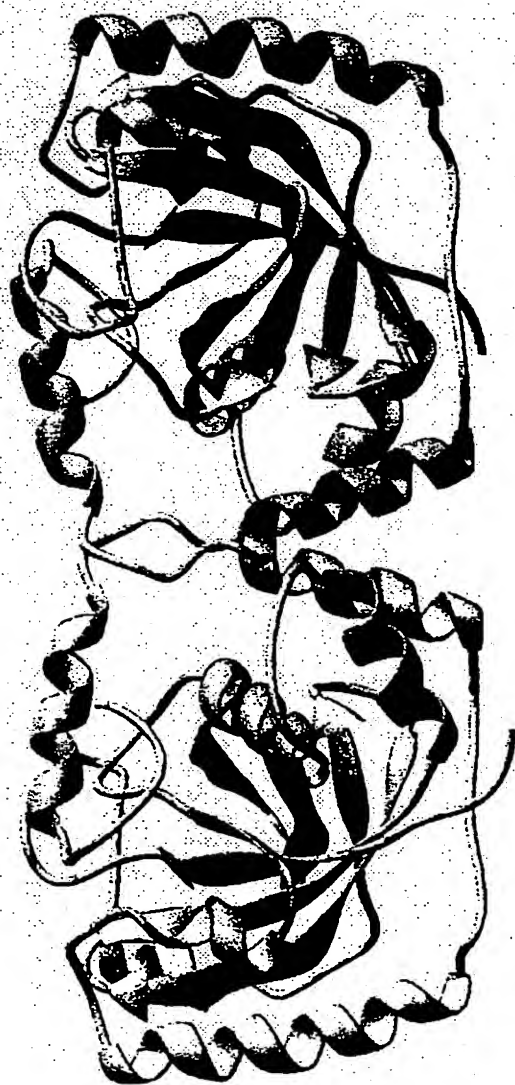


Fig. 28B

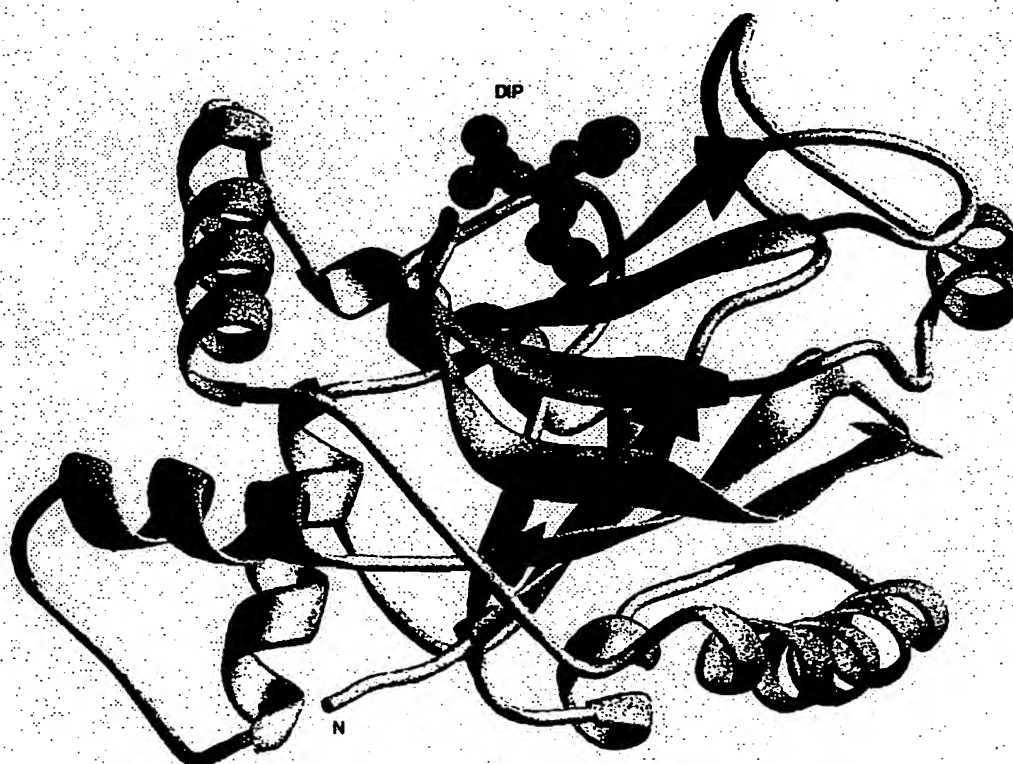


Fig. 29A

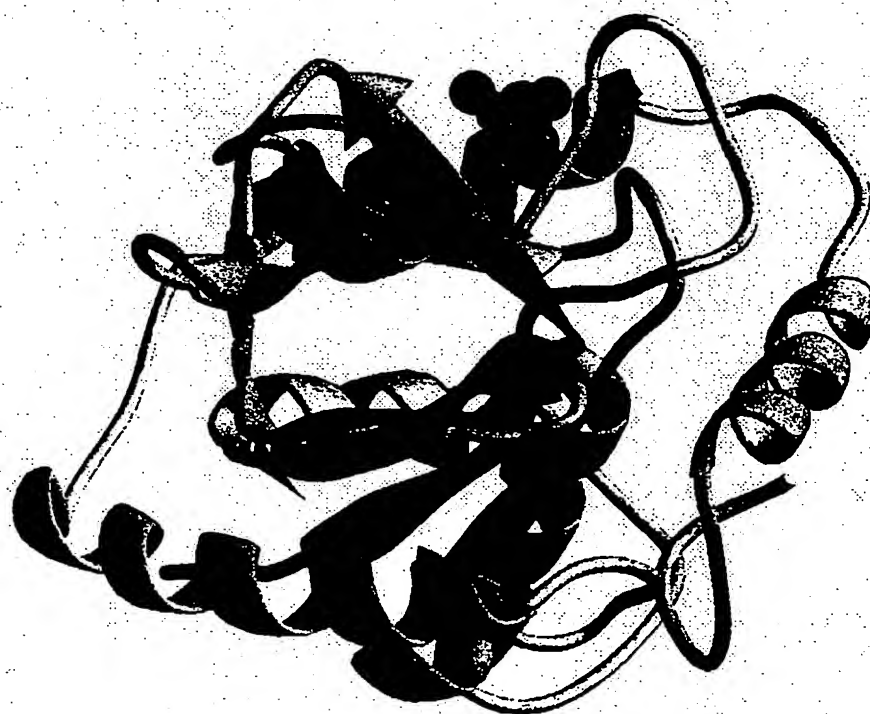


Fig. 29B

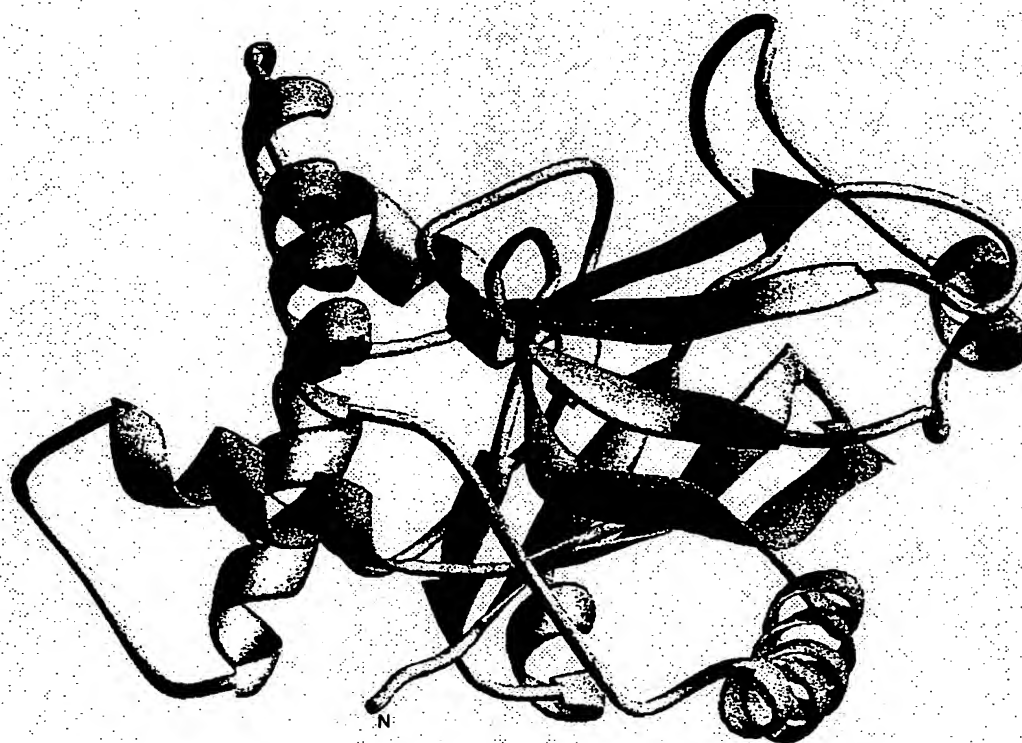


Fig. 29C

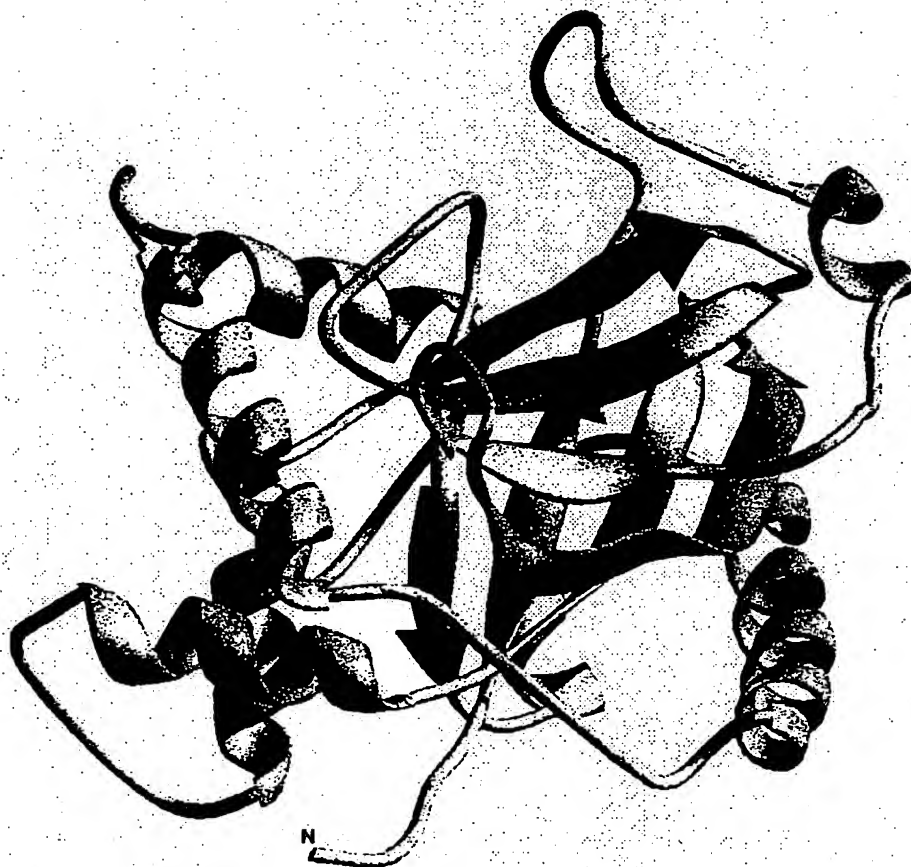


Fig. 30A

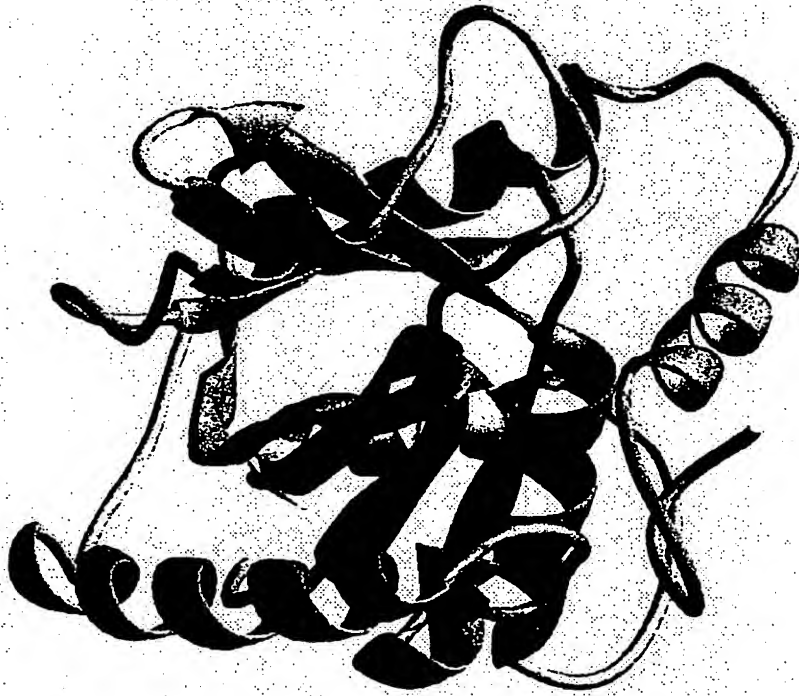


Fig. 30B

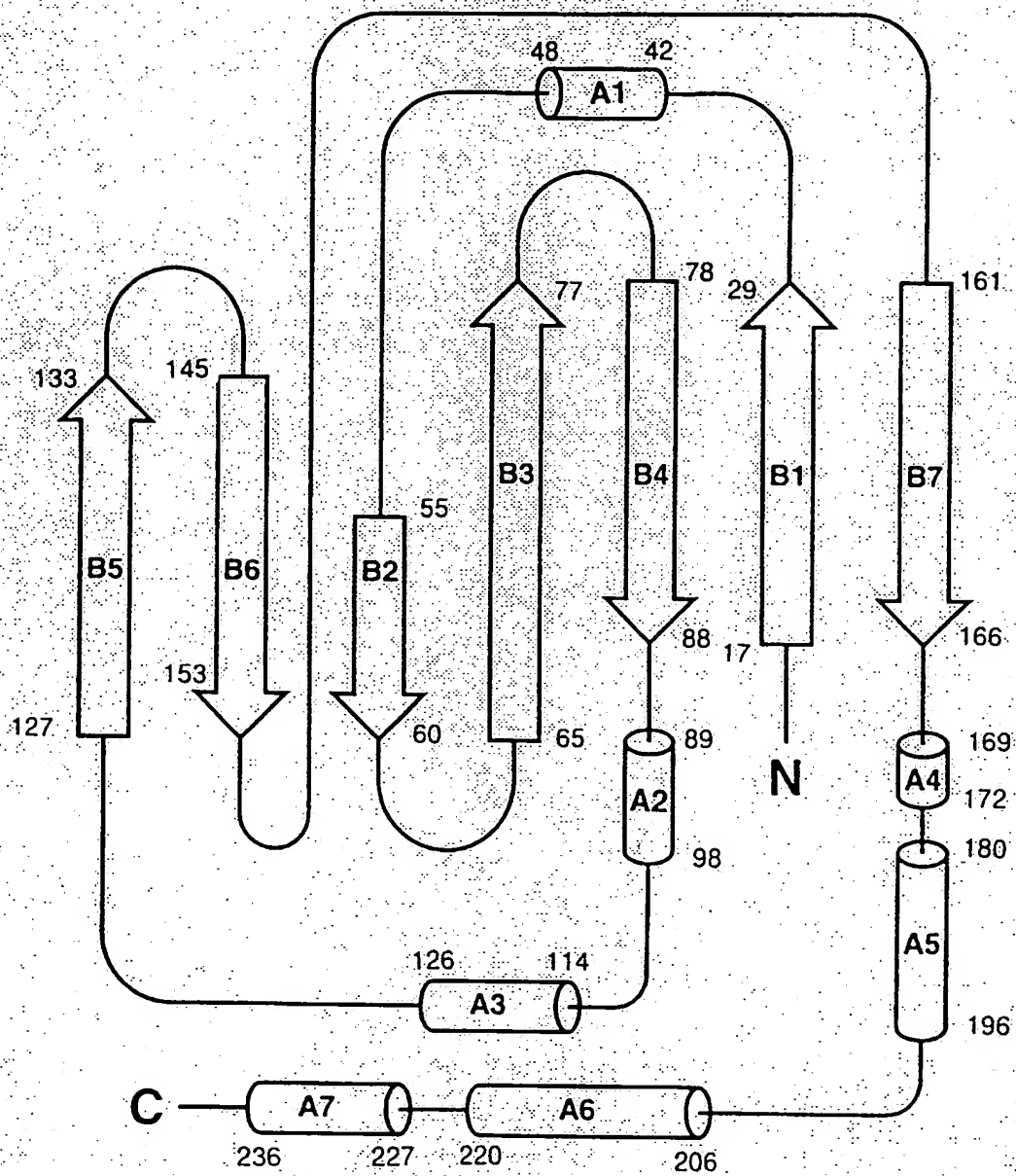


Fig. 31

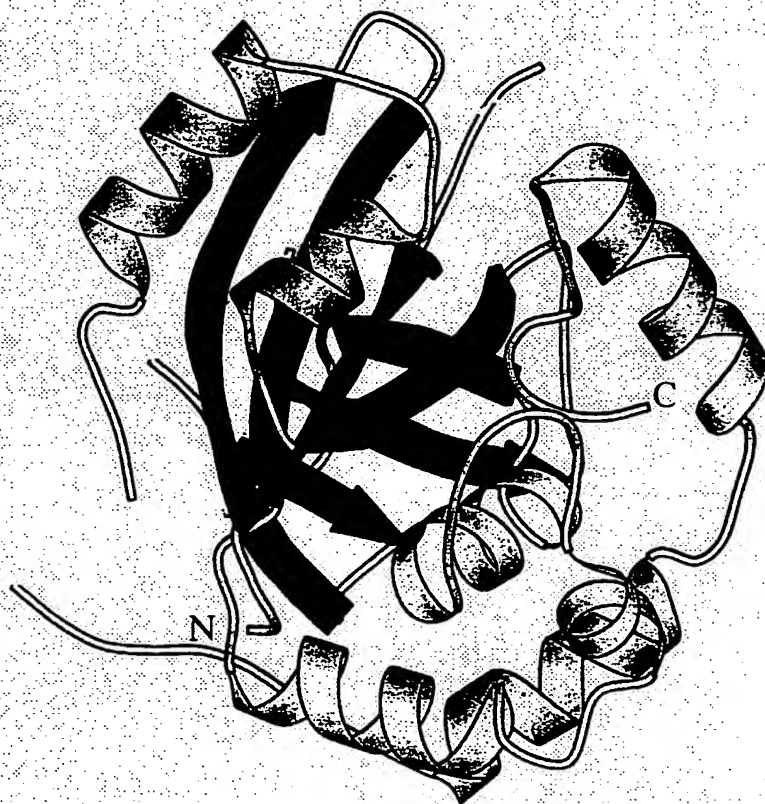


Fig. 32A

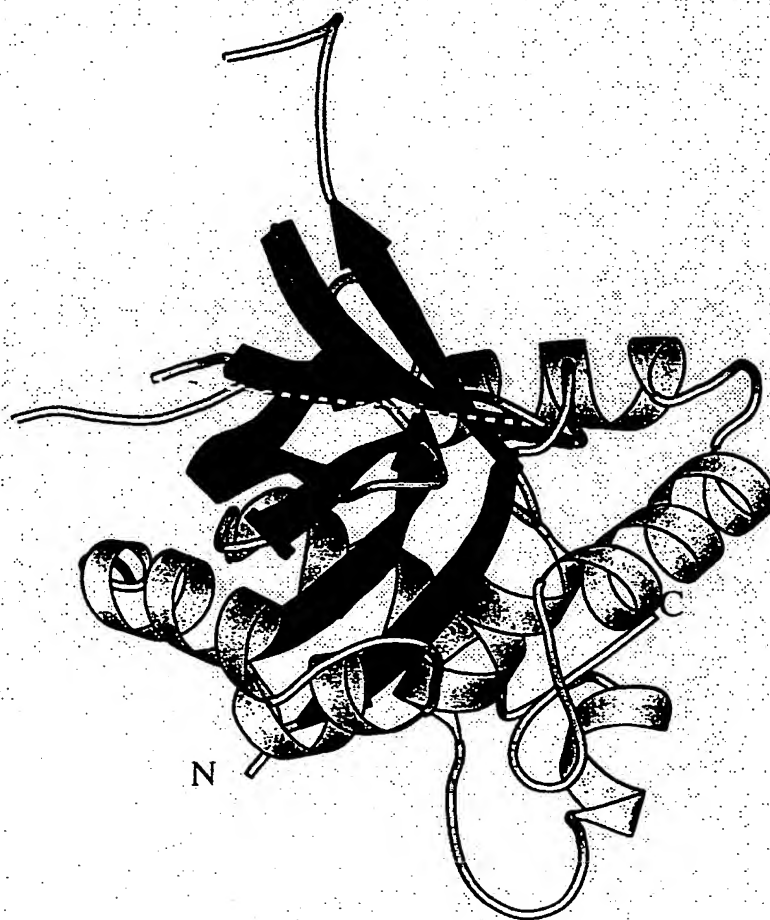


Fig. 32B

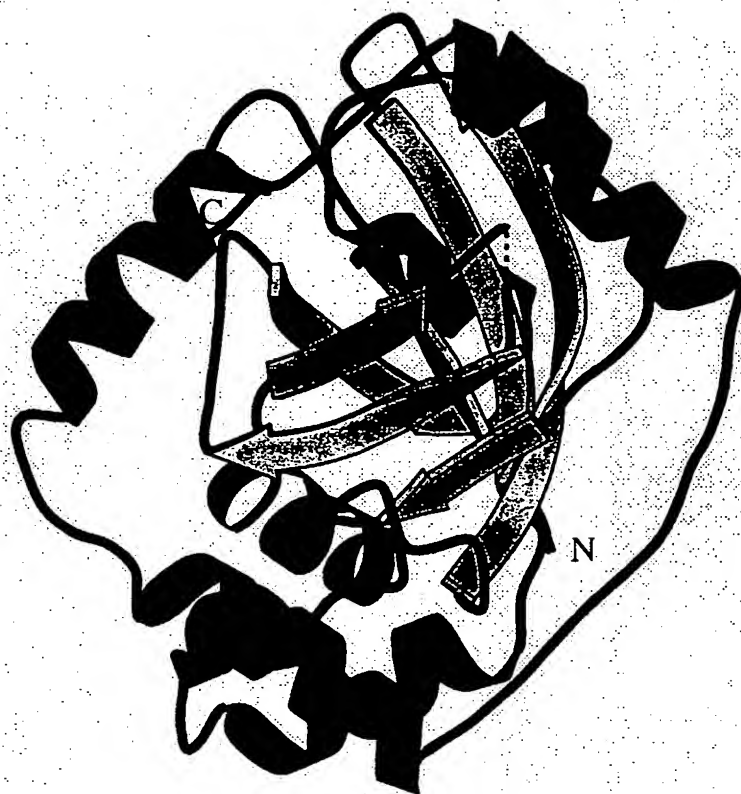


Fig. 33A

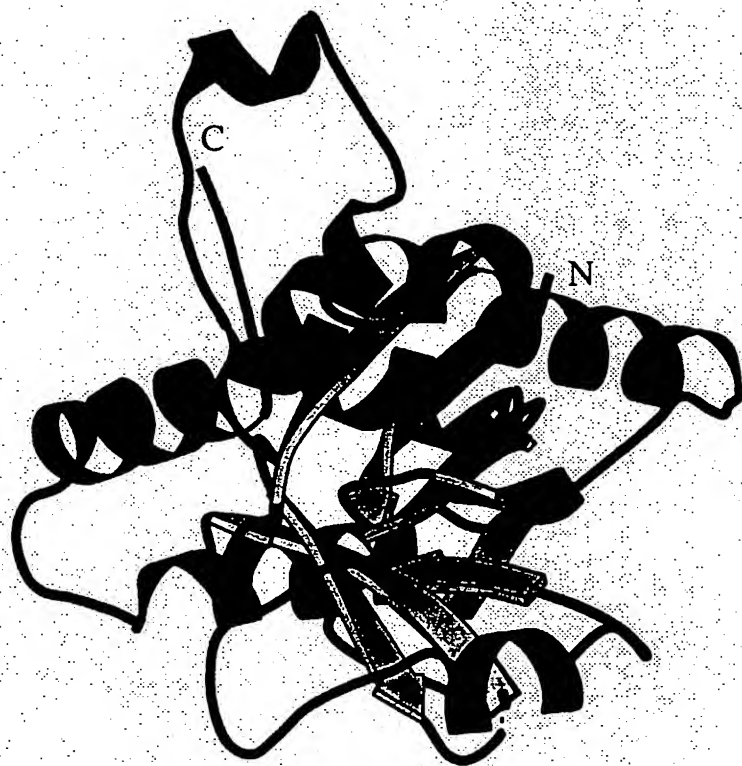


Fig. 33B

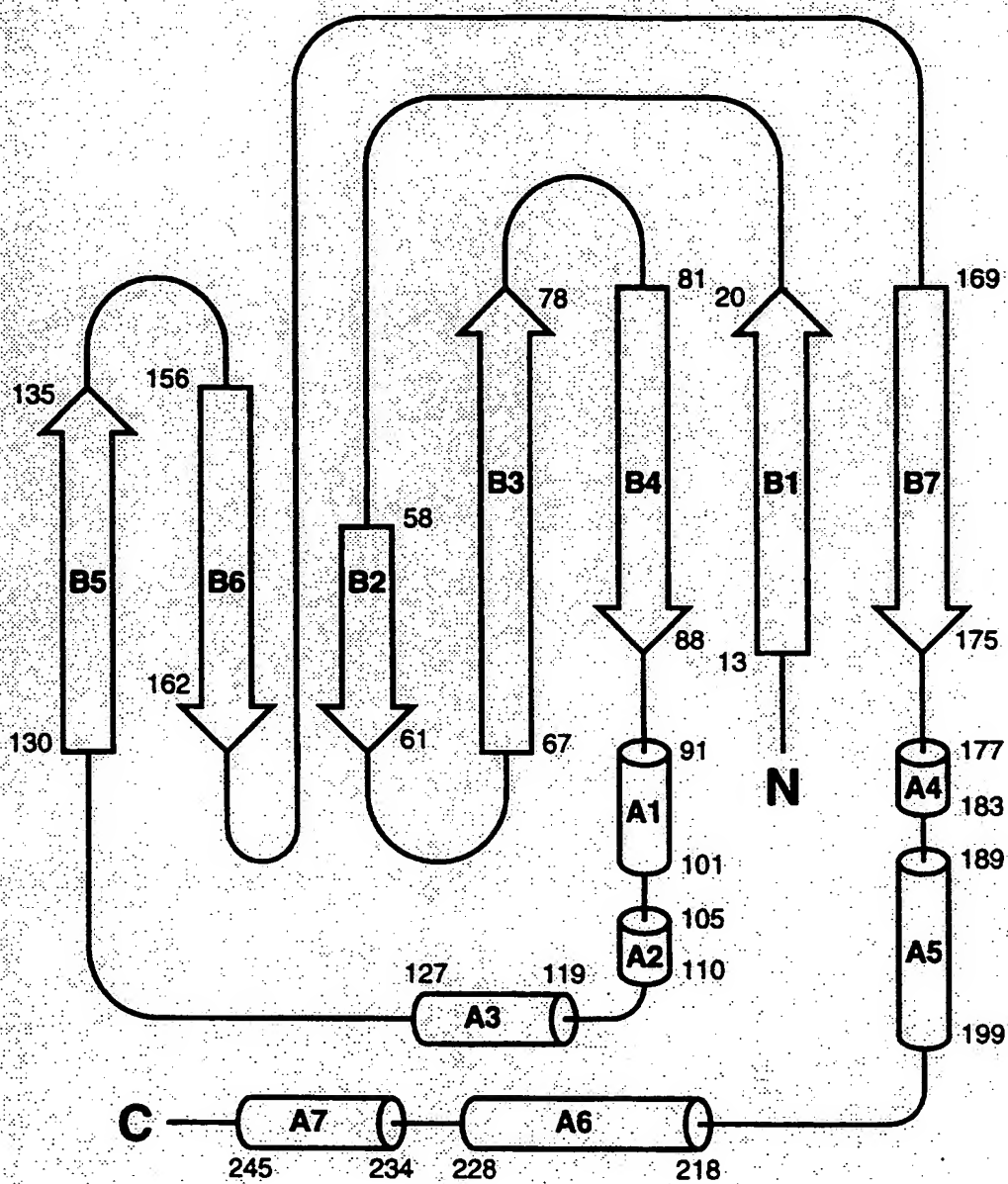


Fig. 34

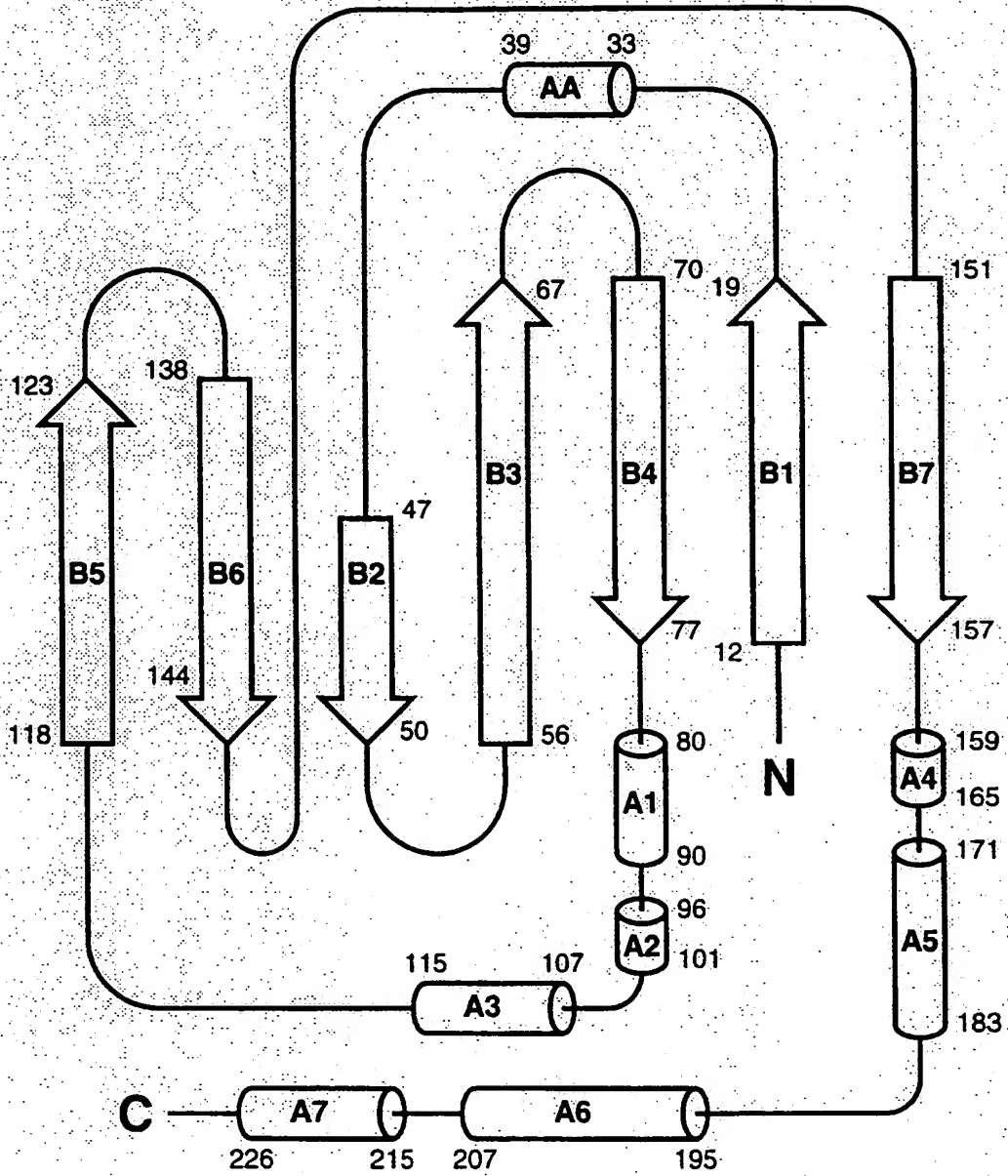


Fig. 35

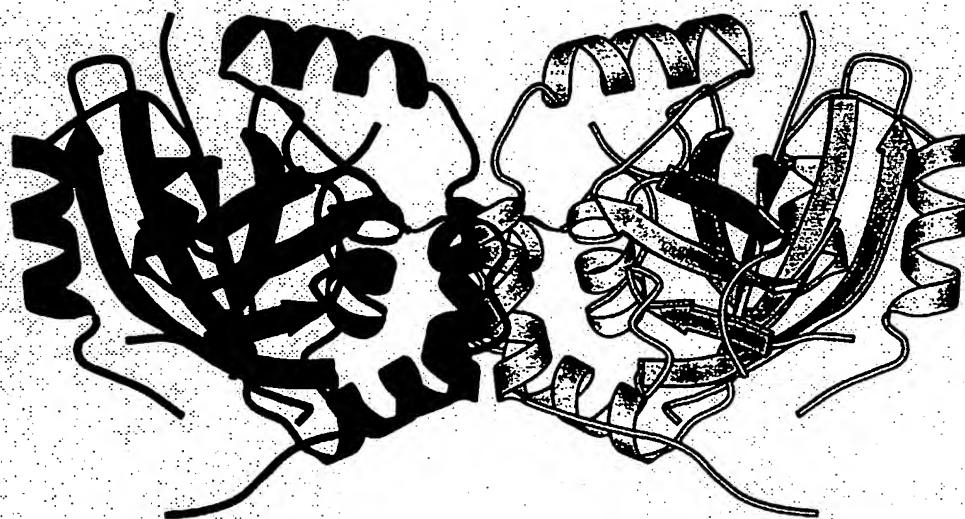


Fig. 36A

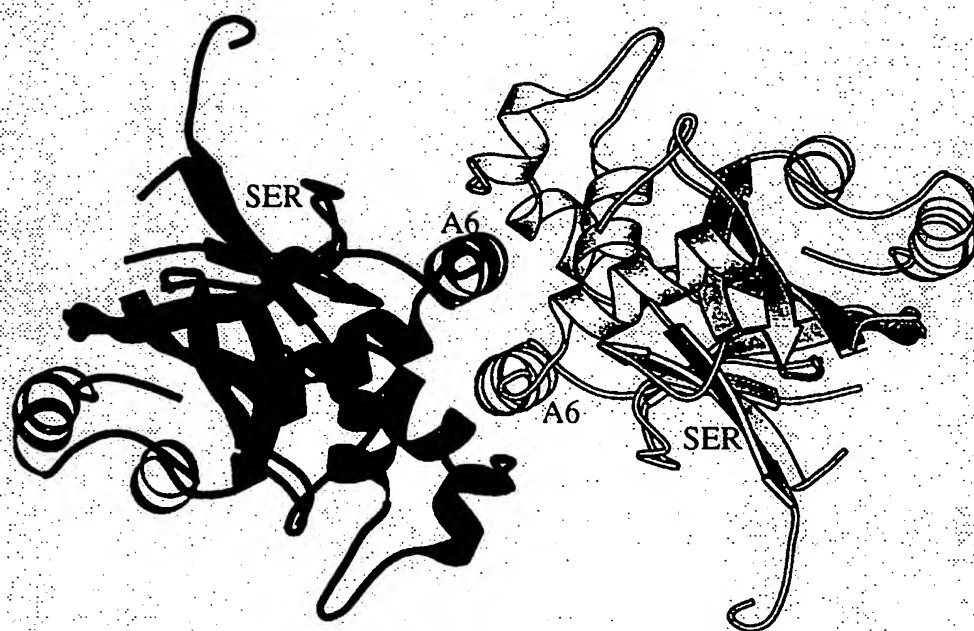


Fig. 36B

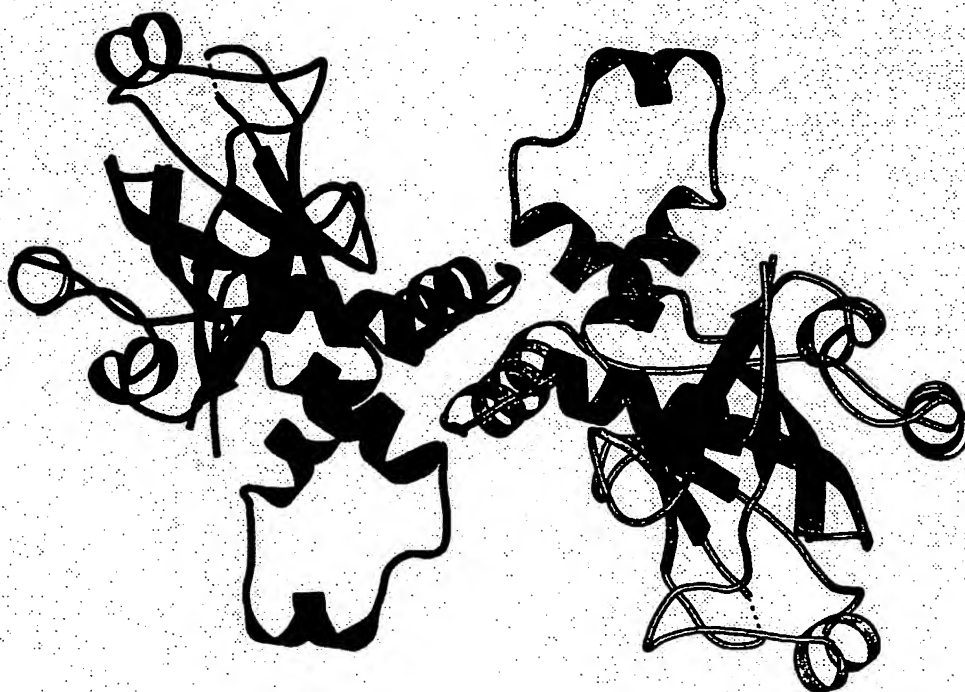


Fig. 37

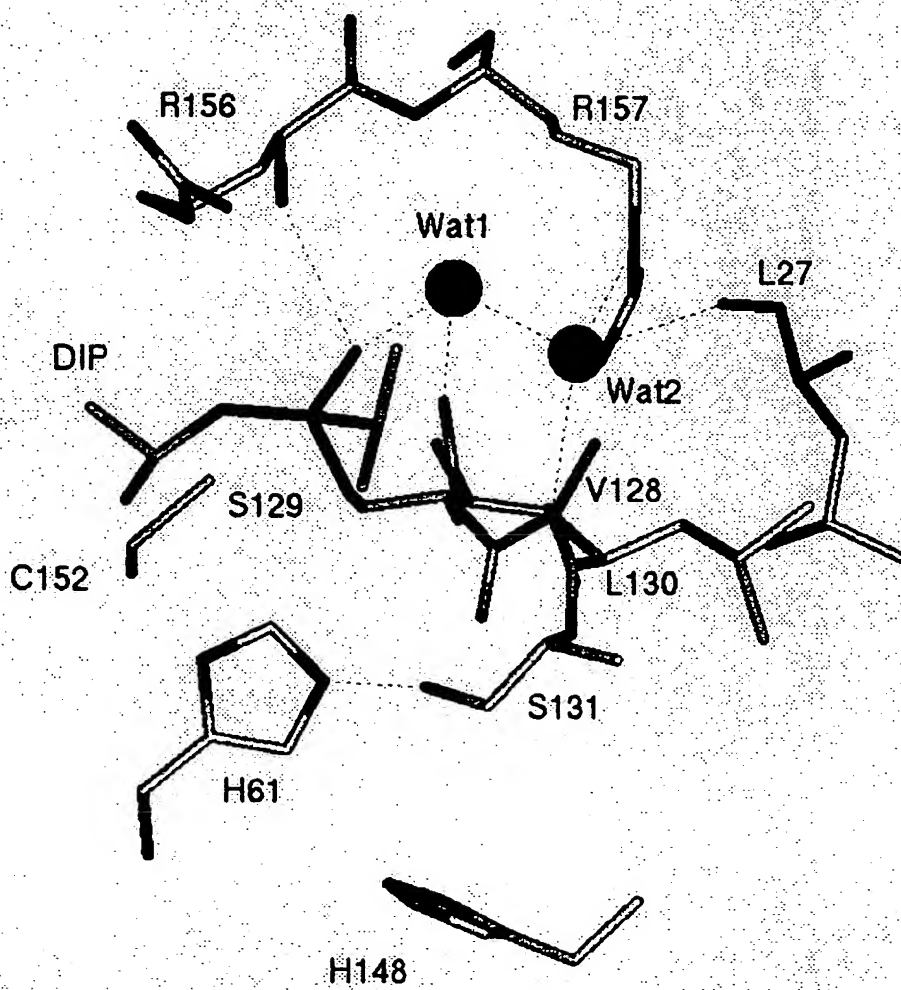
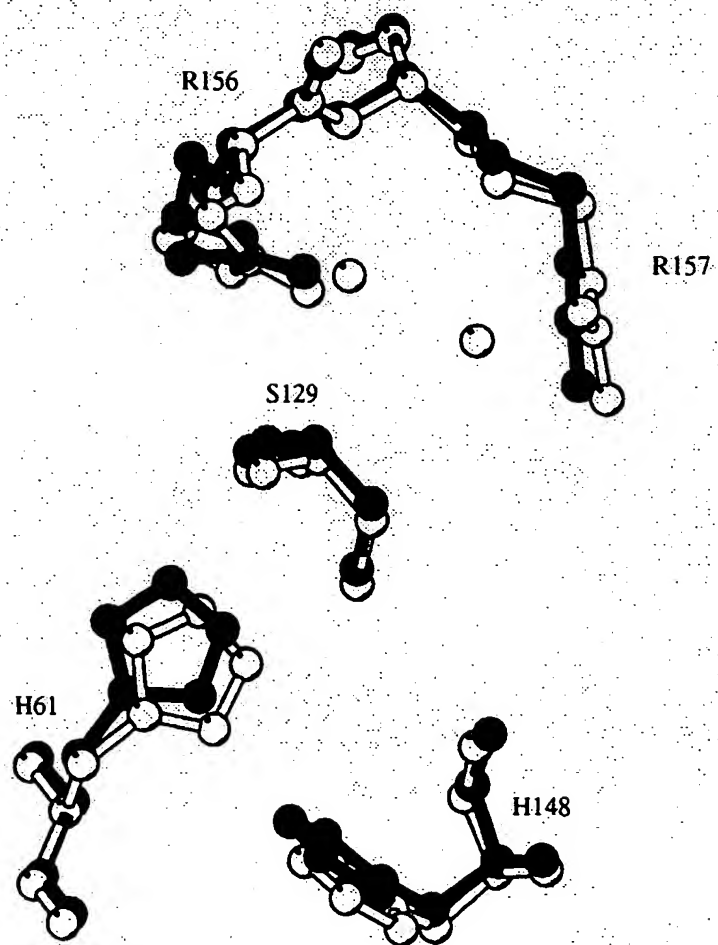


Fig. 38A

Fig. 388



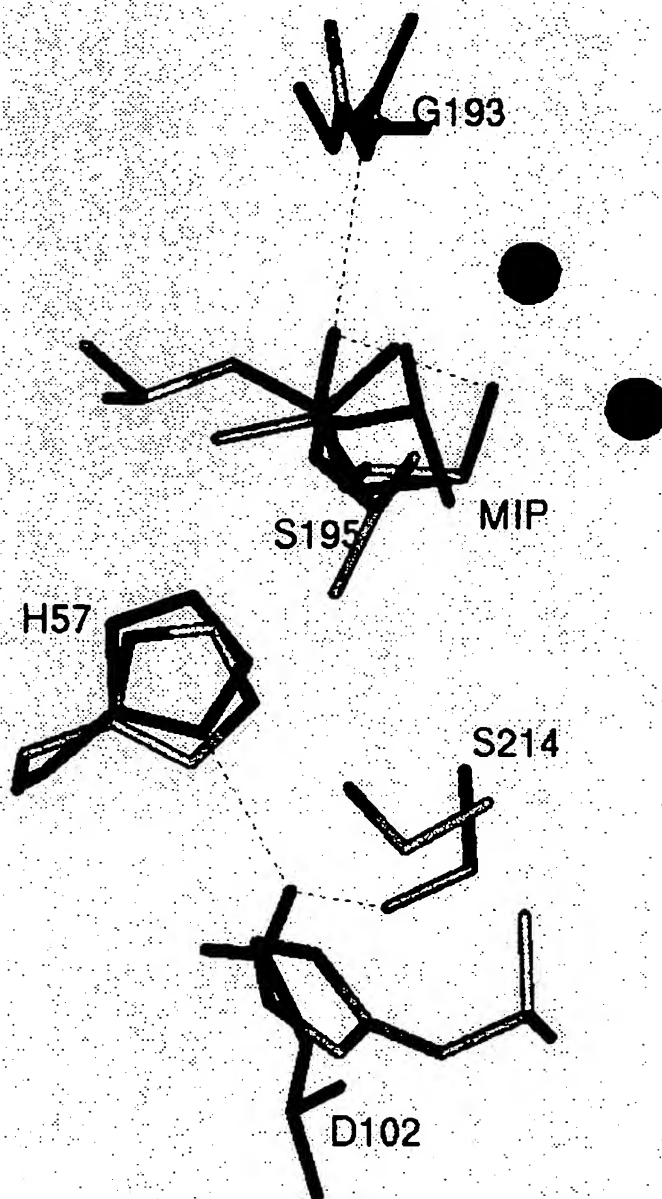


Fig. 38C

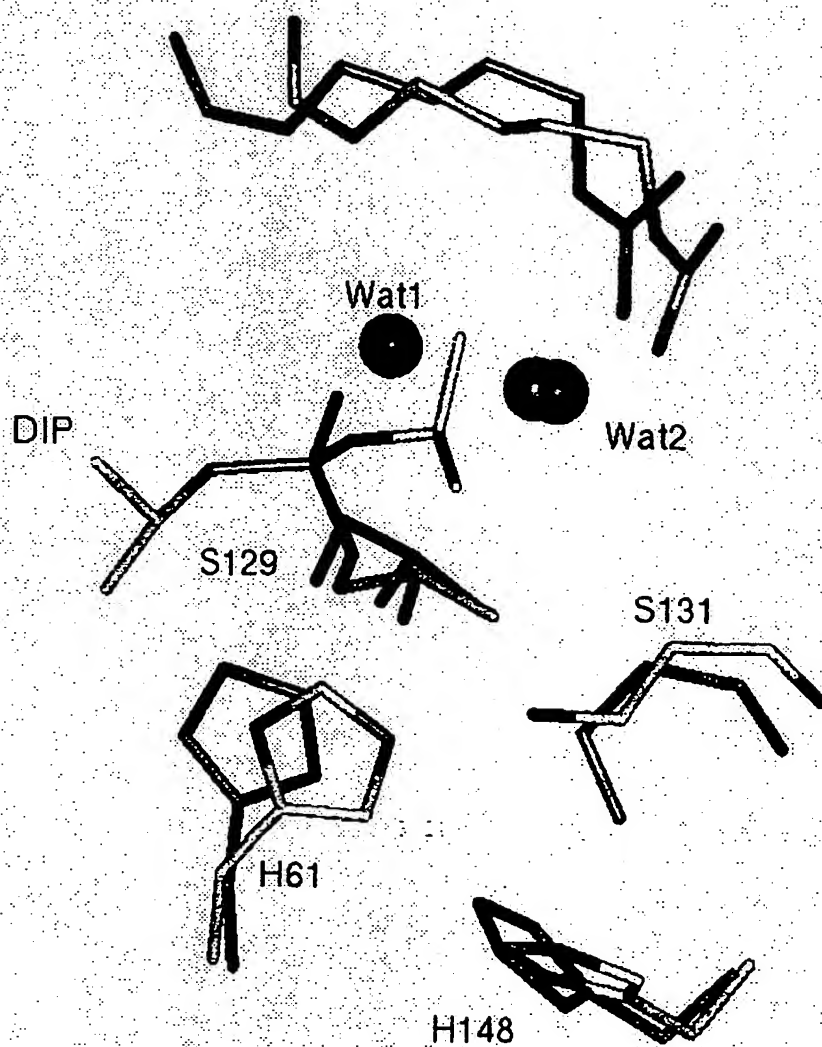


Fig. 380

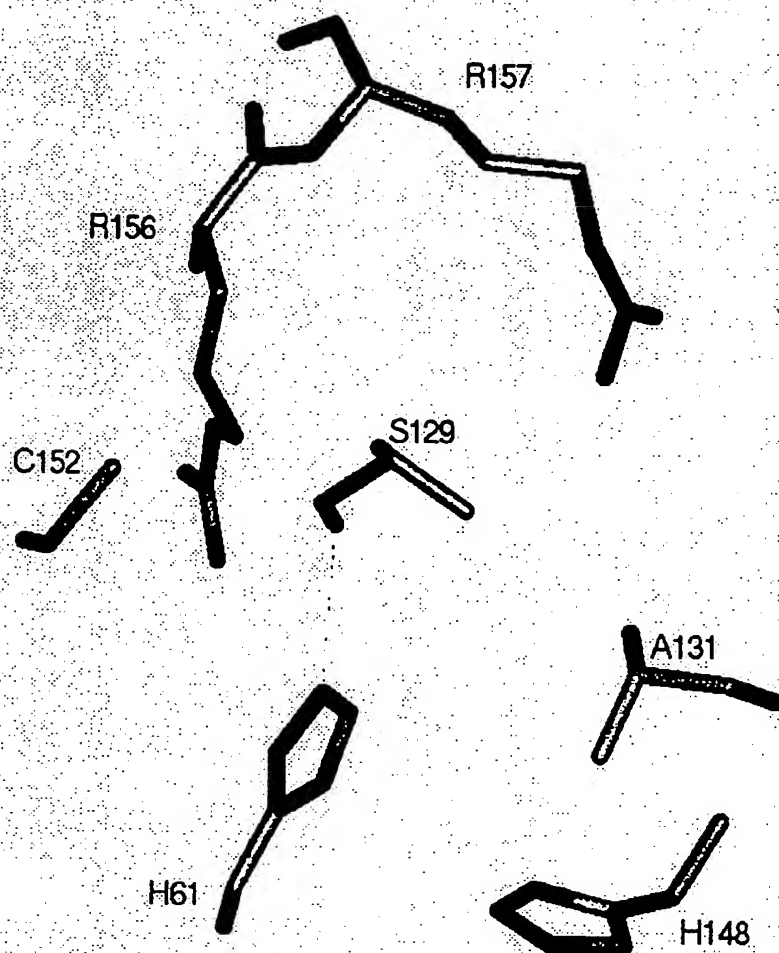


Fig. 39A

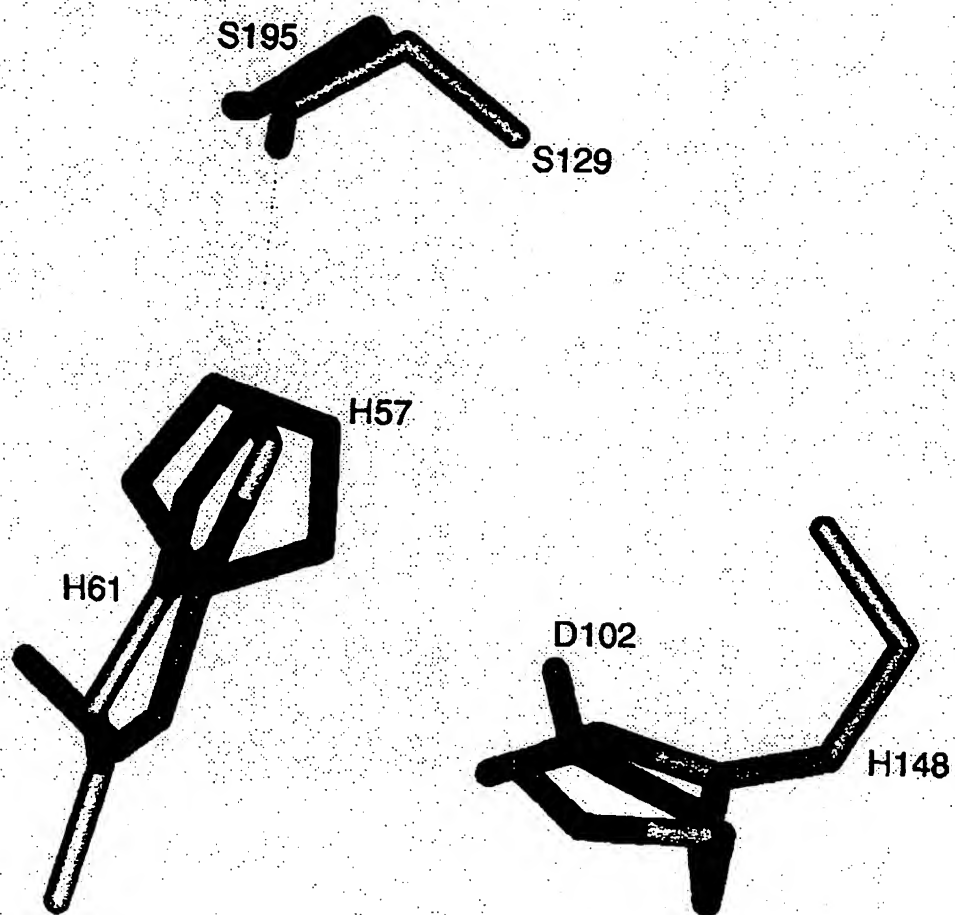


Fig. 39B

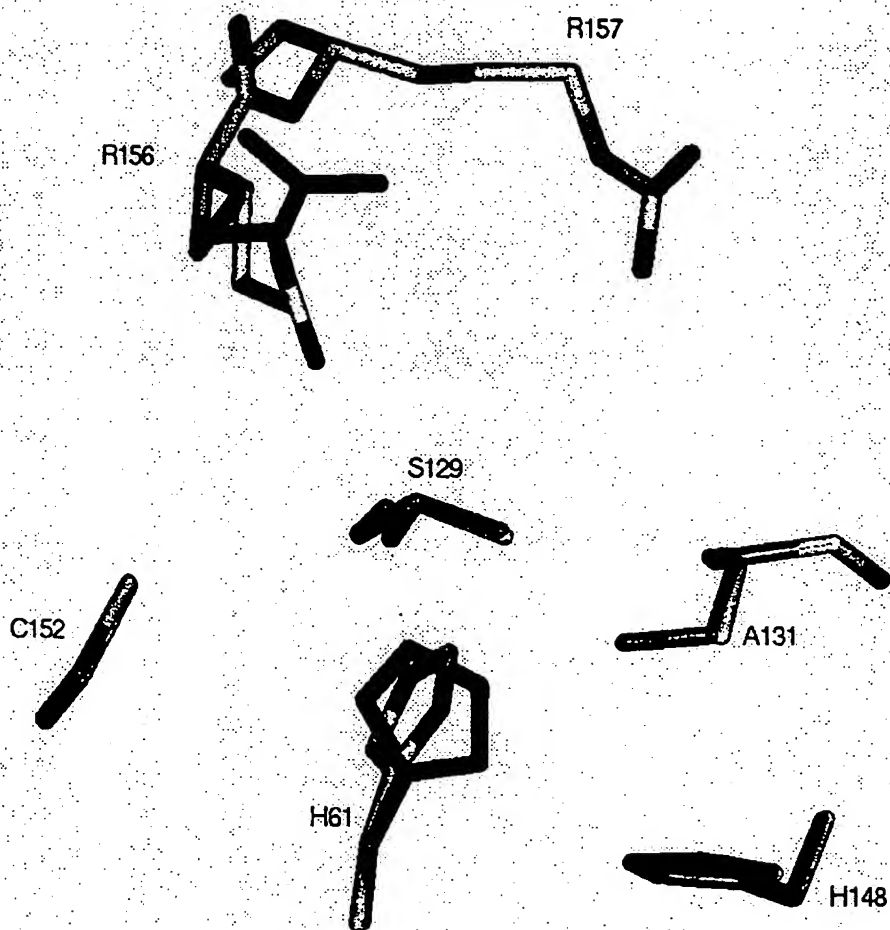


Fig. 39C

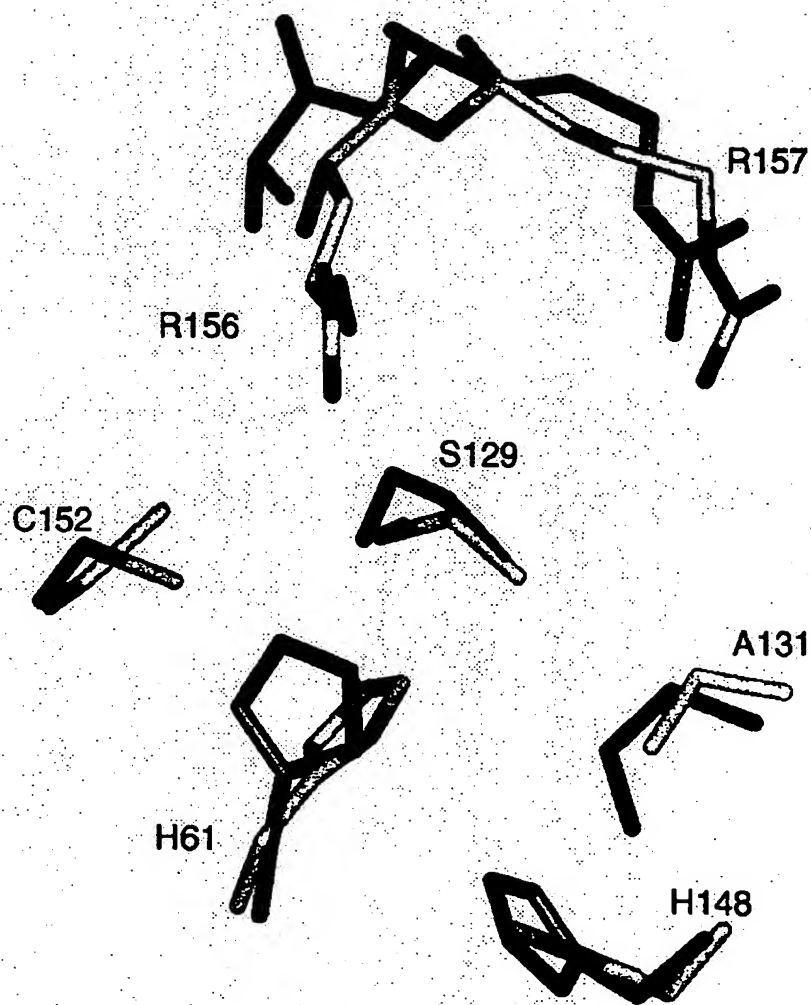
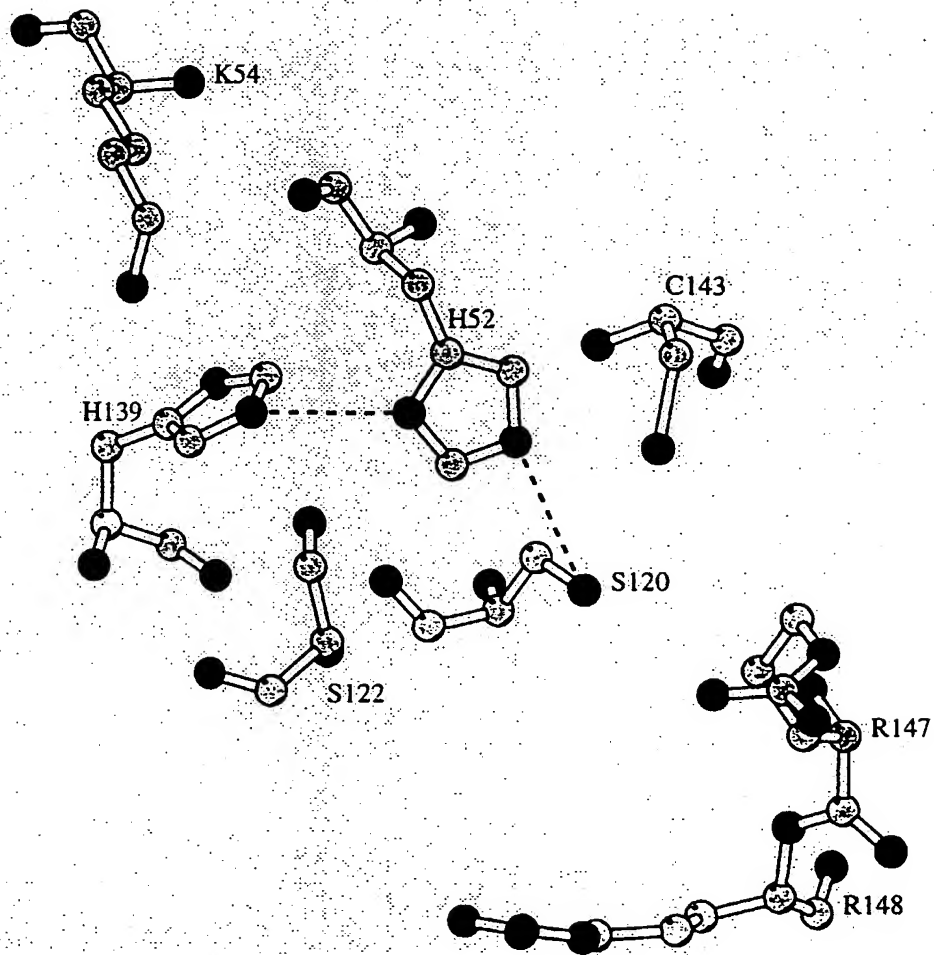
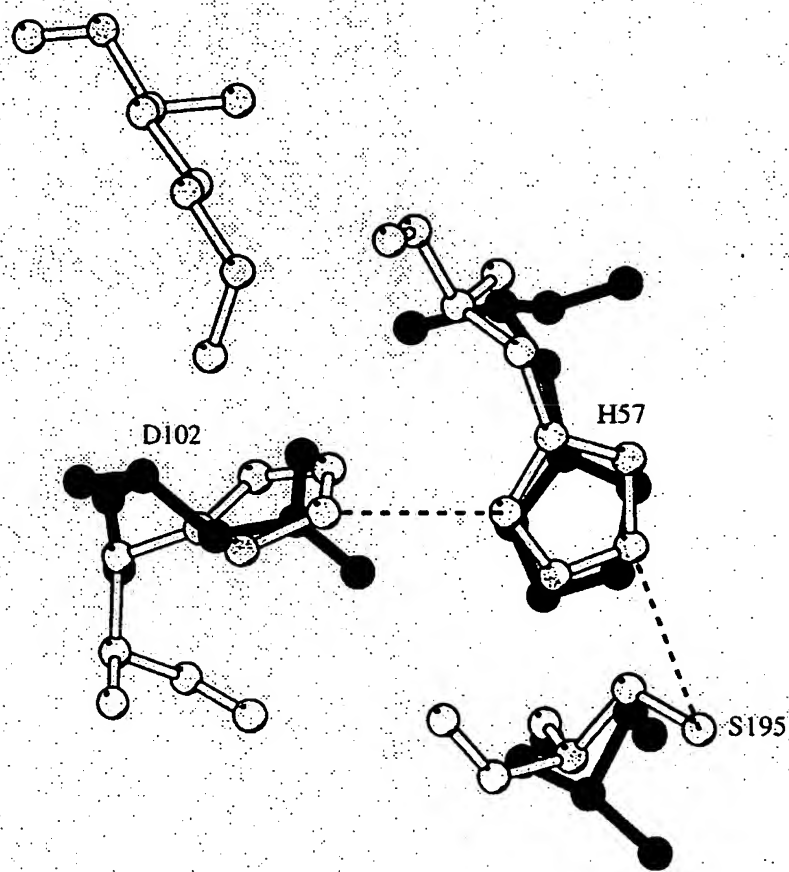


Fig. 39D



VZVP Active Site

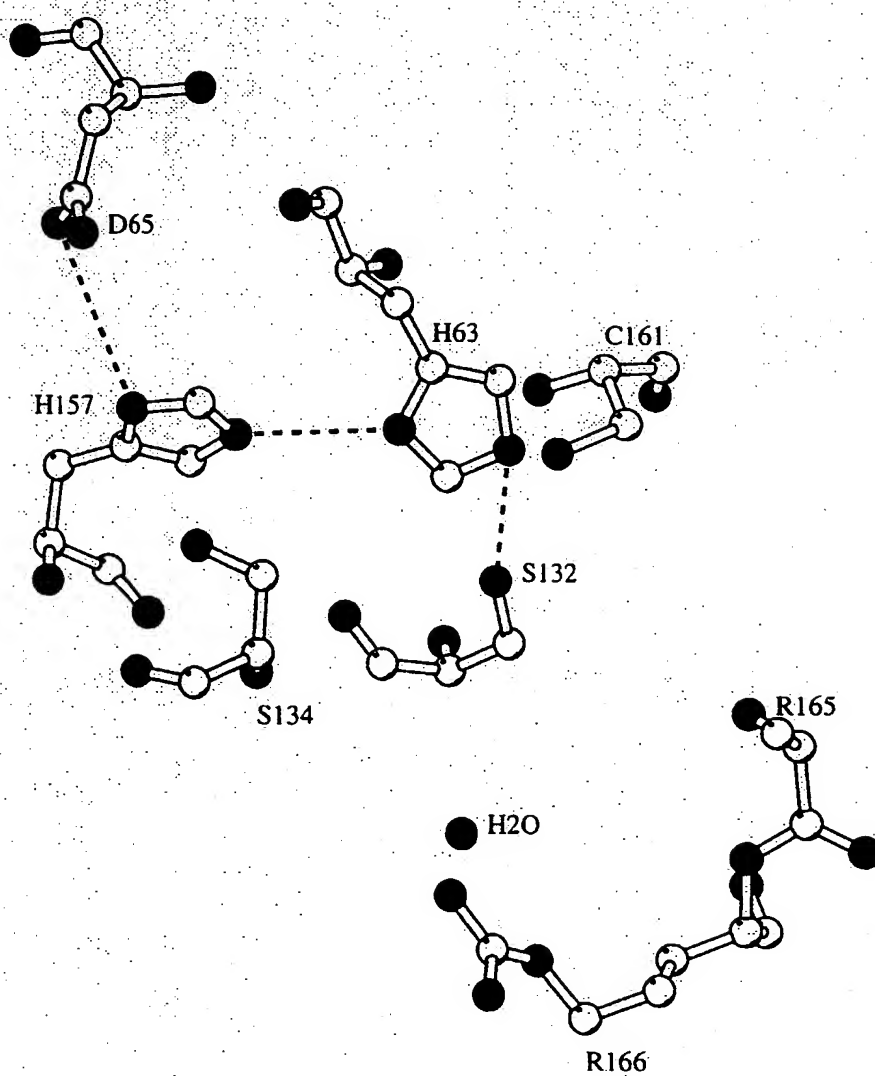
Fig. 40A



Light-VZV, Dark-Trypsin

Fig. 40B

Fig. 41A



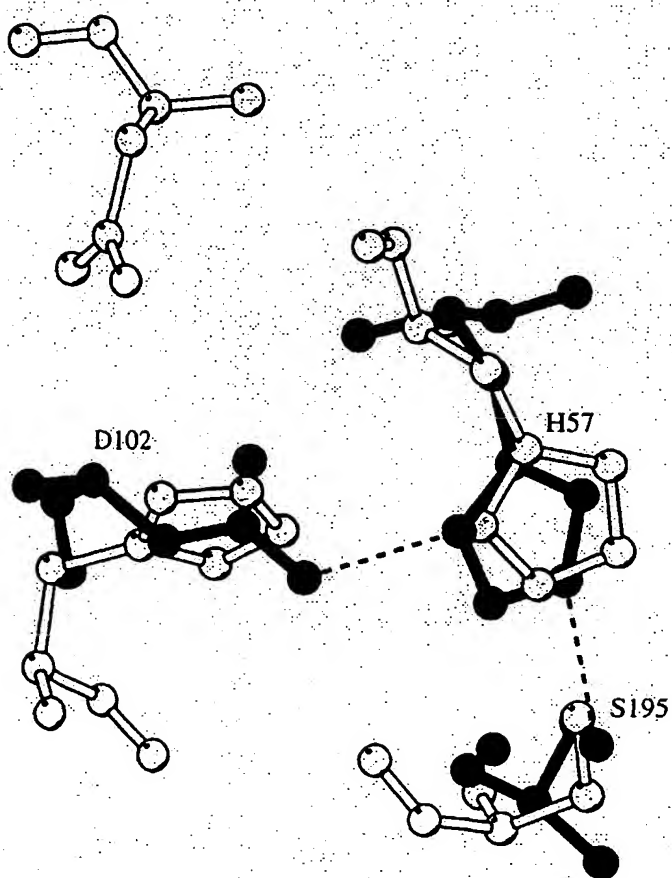


Fig. 418

Figure 42: Structure Determination Statistics

Data Set	Resol'n (Å)	Observed	Unique	Complect (%)	R _{sym}	R _{iso}	# sites	Phasing Power	R _{crullis}
Native	2.5	78502	15788	90.8	0.095	---	---	---	---
KAuCN	3.0	31511	10071	98.2	0.078	15.9	2	1.14	0.74
LuCl ₃	3.0	31104	9964	97.3	0.078	12.4	1	1.51	0.79
PrCl ₃	3.0	31645	10179	99.0	0.090	13.6	1	1.4	0.82
YbSO ₄	4.0	10495	3787	78.7	0.088	14.6	1	2.01	0.72
GdCl ₃	4.0	18308	4268	96.6	0.166	15.7	1	1.56	0.79
SmCl ₃	4.0	25172	4327	97.6	0.114	8.8	1	1.47	0.86

MIR Overall Mean Figure of Merit (15-3.0 Å): 0.62 Å

Overall Figure of Merit After Phase combination: 0.67 Å

Mean Figure of Merit following density modification 100-3.0Å: 0.838 Å

X-PLOR refinement: 10-2.5 Å

No. Reflections Used (F>2σ): 14605

R-factor: 20.5%

No. Protein atoms (non-H): 3364

No. Solvent Atoms: 43

Rms bond length: 0.016 Å

Rms bond angles: 1.919°

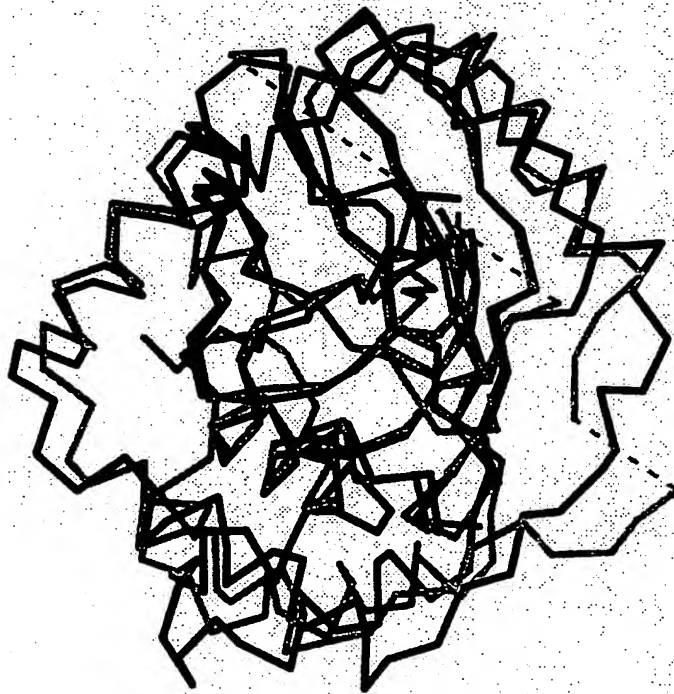
Fig. 43

Data Set	Resolution (Å)	Observed (>1σ)	Unique (>1σ)	Complete (%)	R _m (%)	R _{iso} (%)	# of sites	# of Phasing sites	R _{cullis}	R _c (ano)
Native	2.5	22880	7644	90	6.0	-----	--	---	---	--
MeHgCl	3.2	17566	3932	97	10.1	28.0	5	2.8	0.50	0.92
MeHgCl	3.5	3698	1958	76	19.8	36.5	3	1.4	0.75	--
UO ₂ Ac ₂	3.8	9122	2330	99	23.2	27.5	2	1.1	0.83	--
BakerHg ₂	3.2	14867	4425	97	9.8	30.7	4	1.9	0.68	0.97
LuCl ₃	3.2	9984	3734	95	10.8	23.4	3	2.0	0.63	--
K ₂ PtCl ₄	4.1	3017	1673	79	13.1	25.9	2	1.4	0.77	--
SmCl ₃	3.7	12708	2804	98	13.7	26.3	3	2.4	0.54	0.97

MIRAS Figure of Merit (30 - 3.2 Å): 0.70

XPLOR Refinement:

Resolution included	7.0 - 2.5 Å	# of solvent atoms (non-H)	73
# of reflections used (>1σ)	7193	Mean coordinates error	0.40 Å
R-factor	0.185	Rms bond length	0.017 Å
# of protein atoms (non-H)	1504	Rms bond angle	2.2 degree
(202 amino acids)			



Light-CMV, Dark-VZV, RMSCA 1.3A

Fig. 44

FIG. 45A [SEQ ID NO: 7]

H6(N)VZV:

MGHHHHH SSGHDDDDK MAAEAEENC EALYVAGLYA LYSKDEGELN
 ITPEIVRSAL PPTSKIPINI DHRKDCVVGE VIAIIEDIRG PFFLGIVRCP QLHAVLFEAA
 HSNFFGNRDS VLSPLERALLY LVTNYLPSVS LSSKRLSPNE IPDGNFFTHV ALCVVGRRVG
 TVVNYDCTPE SSIEPFRVLS MESKARLLSL VKDYAGLNKV WKVSEDKLAK
 VLLSTAVNNM LLRDRWDVVA KRRREAGIMG HVYLQA 254

FIG. 45B [SEQ ID NO: 8]

LOA-H6(C) VZV

MAAEAEENC EALYVAGLYA LYSKDEGELN ITPEIVRSAL PPTSKIPINI DHRKDCVVGE
 VIAIIEDIRG PFFLGIVRCP QLHAVLFEAA HSNFFGNRDS VLSPLERALLY LVTNYLPSVS
 LSSKRLSPNE IPDGNFFTHV ALCVVGRRVG TVVNYDCTPE SSIEPFRVLS MESKARLLSL
 VKDYAGLNKV WKVSEDKLAK VLLSTAVNNM LLRDRWDVVA KRRREAGIMG
 HVYLQAHHHH HH 242

FIG. 45C [SEQ ID NO: 9]

LOAS-H6(C) VZV

MAAEAEENC EALYVAGLYA LYSKDEGELN ITPEIVRSAL PPTSKIPINI DHRKDCVVGE
 VIAIIEDIRG PFFLGIVRCP QLHAVLFEAA HSNFFGNRDS VLSPLERALLY LVTNYLPSVS
 LSSKRLSPNE IPDGNFFTHV ALCVVGRRVG TVVNYDCTPE SSIEPFRVLS MESKARLLSL
 VKDYAGLNKV WKVSEDKLAK VLLSTAVNNM LLRDRWDVVA KRRREAGIMG
 HVYLQASHHH HH 243

FIG. 45D [SEQ ID NO: 10]

LOAS-12aa ext H6(C) VZV

MAAEAEENC EALYVAGLYA LYSKDEGELN ITPEIVRSAL PPTSKIPINI DHRKDCVVGE
 VIAIIEDIRG PFFLGIVRCP QLHAVLFEAA HSNFFGNRDS VLSPLERALLY LVTNYLPSVS
 LSSKRLSPNE IPDGNFFTHV ALCVVGRRVG TVVNYDCTPE SSIEPFRVLS MESKARLLSL
 VKDYAGLNKV WKVSEDKLAK VLLSTAVNNM LLRDRWDVVA KRRREAGIMG
 HVYLQASTGY GLARITNVNH HHHH 255

FIG. 45E [SEQ ID NO: 11]

Delta9 LOAS- 12 aa ext H6(C) VZV

M EALYVAGLYA LYSKDEGELN ITPEIVRSAL PPTSKIPINI DHRKDCVVGE VIAIIEDIRG
 PFFLGIVRCP QLHAVLFEAA HSNFFGNRDS VLSPLERALLY LVTNYLPSVS LSSKRLSPNE
 IPDGNFFTHV ALCVVGRRVG TVVNYDCTPE SSIEPFRVLS MESKARLLSL
 VKDYAGLNKV WKVSEDKLAK VLLSTAVNNM LLRDRWDVVA KRRREAGIMG
 HVYLQASTGY GLARITNVNH HHHH 246